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Larry Glasser
Clarkson University

Vladimir Protopopescu
Oak Ridge National Laboratory

Frank Tabakin
University of Pittsburgh

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THE MATHEMATICS OF PRINCIPAL VALUE INTEGRALS AND APPLICATIONS TO NUCLEAR PHYSICS, TRANSPORT THEORY, AND CONDENSED MATTER PHYSICS

K. T. R. DAVIES
*Department of Physics, Duquesne University, Pittsburgh, PA 15282-1503, USA**
and Physics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6373, USA

M. L. GLASSER
Department of Physics, Cora and Bayard Clarkson Science Center, Clarkson University, Potsdam, NY 13676, USA

V. PROTOPOPESCU
Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6364, USA

FRANK TABAKIN
Department of Physics & Astronomy, University of Pittsburgh, Pittsburgh, PA 15260, USA

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A review of developments in the mathematics and methods for principal value (PV) integrals is presented. These topics include single-pole formulas for simple and higher-order PVs, simple and higher-order poles in double integrals, and products of simple poles in general multiple integrals. Two generalizations of the famous Poincaré–Bertrand (PB) theorem are studied. We then review the following topics: dispersion relations for the advanced, retarded, and causal Green's functions; Titchmarsh's theorem; applications of the PB theorem to two- and three-particle loop integrals; and the R and T matrix formalism. Also, various applications of the PV methods to nuclear physics, transport theory, and condensed matter physics are studied. In the appendices several methods for evaluating PV integrals, including the Haftel-Tabakin procedure for calculating the R and T matrices, are reviewed.

1. Introduction

In recent years there has been a resurgence of interest in applications of PV methods to intermediate-energy nuclear physics (see Refs. 12, 13, 16, 46, 52 and 60). Most of these studies focus on numerical calculations using various response functions or "loop integrals", which arise from nucleon-delta-pion interactions. Such a response

*Present address

function, involving a product of two single-particle Green's functions, then appears as a *self-energy correction* which is inserted into an *external* propagator, as shown in Fig. 1.

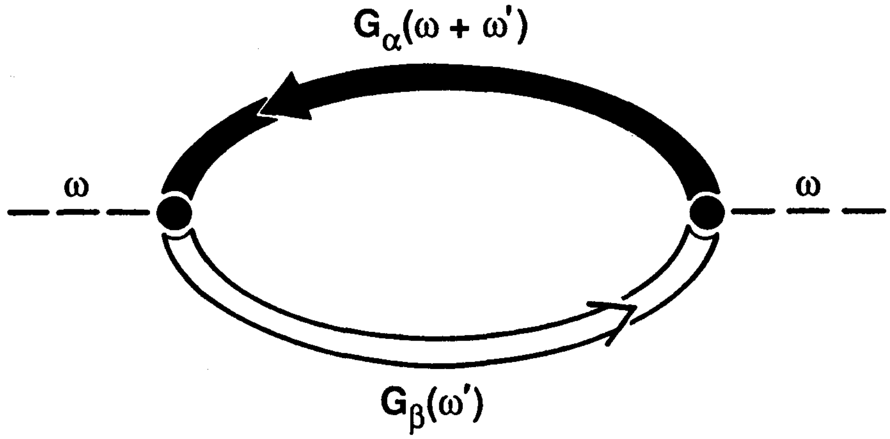

Fig. 1. Feynman diagram for a two-propagator loop integral. The loop is imagined to be inserted, essentially as a self-energy correction, into an external propagator (which is illustrated in the diagram by the dotted line).[12,52]

If one examines the dispersion relations for a general finite-temperature loop integral, one finds that its real and imaginary parts are related by an expression that involves two *PV terms in a double integral.*[12,52] Then, in order to simplify this expression, it is usually necessary to *reverse the order of integrations* in the double integral, an operation that is most elegantly handled using the *PB theorem* (see Refs. 2, 12, 15, 48, 52, 57 and 60). These manipulations are discussed in Sec. 3 of this paper, in which we also treat the dispersion relations for the finite-temperature *three-particle loop integral.*[12] (See Fig. 2.) Then, some results of numerical calculations of two-particle loop integrals in intermediate-energy nuclear physics are reviewed in Sec. 5 of the paper.

There have also been many applications of PV methods in nuclear physics,[29,41] condensed matter physics[25] and transport theory.[8,36] Moreover, the PB theorem was used in a study, in momentum space, of the quantum mechanical reflection and transmission at a potential step.[35] Also, recently[39] certain PV logarithmic integrals, which arise in the plasma energy of an electron gas, can be evaluated using a generalized dilogarithm. Such research, of course, is only a small sampling of all of the many applications of PV methods in physics, applied mathematics, and engineering.

Thus, there has been new interest in the mathematics of PV integrals (see Refs. 2, 11, 12, 15, 44, 47, 48, 57 and 60), and in analytic and numerical methods used to

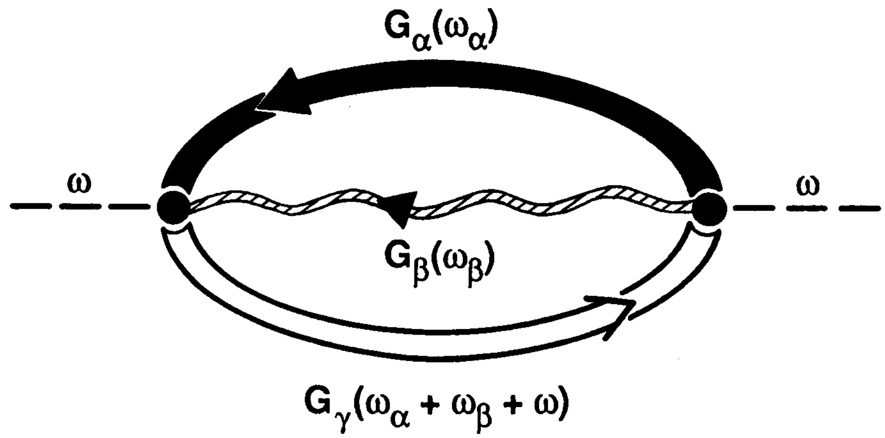

Fig. 2. Feynman diagram for a three-propagator loop integral. Again, the dashed line represents an external propagator into which the loop is inserted.

calculate such integrals (see Refs. 10, 11, 13, 15, 17, 29, 47, 54, 55 and 60).

The purpose of this paper is threefold:

(i) to review the mathematics and methods of PV integrals (Sec. 2 and Appendices A, B and C);
(ii) to discuss the application of PV methods to general techniques commonly used in physics, mathematical physics and applied mathematics, such as dispersion relations and various Green's functions (Secs. 3 and 4; Appendix B);
(iii) to review more detailed applications of the PV formalism in nuclear physics, transport theory and condensed matter physics (Secs. 5–7, respectively).

Our review of PV methods and applications is by no means exhaustive. The literature on this subject is simply too vast to be covered in a single review paper. However, we do believe that the papers referenced and the topics and examples presented here are *representative* of the most important kinds of PV studies occurring in mathematical physics. Moreover, the examples that we address here largely involve *numerical* treatment of PV integrals as opposed to earlier studies in which PVs were evaluated analytically, often by complex variable calculus.

Typically, most physicists learn to manipulate and evaluate simple PV integrals early in their professional careers. Of particular importance are infinite-limit integrals containing a single pole, which can be evaluated by complex variable theory if the integrand contains fairly simple analytic functions.[11,47] However, such integrals can usually be evaluated almost mechanically, without any real understanding of the *true meaning* of the PV; i.e. one wishes to know the *precise interpretation* of the equation

$$I(a) = \mathcal{P} \int \frac{g(x)}{(x-a)} dx, \tag{1.1}$$

where the integration limits can either be finite or infinite, $g(x)$ is "well-behaved" over the region of interest, and $\mathcal{P}$ denotes the PV operation.

We believe that there are a number of misconceptions regarding the fundamental meaning of PV. Also, for many applications, it is crucial to understand the PV operation. In particular, for developing accurate numerical methods to evaluate PV integrals, an intimate familiarity with basic definitions is absolutely essential (see Refs. 10–13, 17, 29, 47, 54, 55 and 60). In Sec. 2 of this paper, we attempt to clarify certain problems associated with misconceptions, misinformation, or plain mistakes about the PV operation.

The first common misconception about the PV is that, in an equation like (1.1), one is somehow evaluating a contribution from the pole. This is nonsense, of course, since in most cases the pole contribution is infinite. (Whether the integral in Eq. (1.1) *without the PV symbol* actually diverges depends on the limits of integration and the precise form of $g(x)$.) In Eq. (1.1) what one is evaluating is the integral over the entire range of integration, *except for an infinitesimally small region near the pole.* In fact, a fundamental definition of the PV that is strongly suggested in the literature is that the PV is the "convergent part" of an otherwise divergent integral (see Refs. 11, 15, 17, 24 and 37). While this definition may be almost trivial for simple, single pole formulas (like Eq. (1.1)) its extension to more complicated cases requires considerable justification.

A second misconception about the mathematics of PV integrals is that the basic definition is limited to an isolated simple pole, as in Eq. (1.1). In fact, the PV idea can be usefully extended to higher-order poles[11,15]; e.g.

$$I^{(n)}(a) = \mathcal{P}\int \frac{g(x)}{(x-a)^n}dx\,, \quad n > 1\,, \tag{1.2}$$

or to two or more PVs occurring in a multiple integral; e.g.,

$$I(a) = \mathcal{P}\int \frac{dx}{(x-a)}\int \frac{dy}{(y-x)}g(x,y)\,, \tag{1.3}$$

where again the limits of integration can either be finite or infinite. Equation (1.3) is the type of integral, previously mentioned, to which the PB theorem and its generalizations apply (see Refs. 2, 12, 15, 48, 52, 57 and 60).

One important "spinoff" of the PB theorem is a generalization of the well-known equation[44]

$$(x-a+i\varepsilon)^{-1} \underset{\varepsilon\to 0}{\longrightarrow} \frac{\mathcal{P}}{x-a} - \pi i\delta(x-a) \tag{1.4}$$

to a double product like

$$(x-a+\ i\varepsilon_1)^{-1}(x-b+i\varepsilon_2)^{-1}.$$

Then, as $\varepsilon_1, \varepsilon_2 \to 0$ we find that

$$(x-a+i\varepsilon_1)^{-1}(x-b+i\varepsilon_2)^{-1} \neq \left[\frac{\mathcal{P}}{x-a} - \pi i\delta(x-a)\right]\left[\frac{\mathcal{P}}{x-b} - \pi i\delta(x-b)\right]. \tag{1.5}$$

The *correct* relation is given by[12,49]

$$(x-a+i\varepsilon_1)^{-1}(x-b+i\varepsilon_2)^{-1} \underset{\varepsilon_1,\varepsilon_2\to 0}{\longrightarrow} \left[\frac{\mathcal{P}}{(x-a)} - \pi i\delta(x-a)\right]\left[\frac{\mathcal{P}}{(x-b)} - \pi i\delta(x-b)\right] + \pi^2\delta(x-a)\delta(x-b). \tag{1.6}$$

The difference between Eqs. (1.5) and (1.6) arises from the PB theorem. Equation (1.6) was recently used in Ref. 35.

There is one final refinement of the PV definition that needs to be mentioned. For *finite-limit* PV integrals we can take advantage of certain "*quadratures*" in order to evaluate the integrals.[15] In particular, assume the existence of a quadrature for the *indefinite* integral

$$F_a^{(n)}(x) = \int \frac{g(x)}{(x-a)^n}dx, \tag{1.7}$$

which in principle always exists. Then, it can be shown that

$$\mathcal{P}\int_b^c \frac{g(x)}{(x-a)^n}dx = F_a^{(n)}(c) - F_a^{(n)}(b), \tag{1.8}$$

a result that is valid whether the point a lies on the interval between b and c, or outside that interval. In other words, the PV of the integral is simply the differences of the quadratures, obtained by ignoring the singularity and "blindly integrating through it". Once again, we see that the PV is the convergent part of the integral.

With these preliminaries, we next begin Sec. 2, containing the formal PV definition and its generalizations. The mathematics of PV integrals is covered in Sec. 2, and a number of important applications are reviewed in Secs. 3–7. In Sec. 8 we give a brief summary of this paper.

In Appendix C we present a remarkable property of PV integrals, virtually unknown, that greatly extends the number of one-dimensional PV integrals that can be evaluated exactly.

2. Principal Value Integrals

2.1. *Single-pole formulas for principal value integrals*

2.1.1. *General formulas*

First, we explain our terminology. A *single pole expression* is a single integral whose integrand is given by

$$G_n(x) = \frac{g(x)}{(x-a)^n}; \quad n \geq 1, \tag{2.1}$$

where x is the integration variable, a is a constant, and n is an integer. Then, a *simple pole* occurs for

$$n = 1, \tag{2.2a}$$

while a *higher-order pole* occurs for

$$n > 1, \tag{2.2b}$$

and we also say that the pole is of order n. We will assume that the function $g(x)$ is "well-behaved" in the integral. More precisely, it is assumed that the function and its first $n-1$ derivatives are finite and continuous over the range of integration. (For most cases of physical interest, $g(x)$ and *all* of its derivatives will be finite and continuous over the range.)

For a simple pole, the fundamental definition of the PV is[11,44]

$$\mathcal{P}\left(\frac{1}{x-a}\right) = \lim_{\varepsilon\to 0^+}\left[\frac{(x-a)}{(x-a)^2+\varepsilon^2}\right], \tag{2.3}$$

while for higher-order poles, we have

$$\mathcal{P}[(x-a)^{-n}] = \frac{(-)^{n-1}}{(n-1)!}\lim_{\varepsilon\to 0^+}\left\{\frac{d^{n-1}}{dx^{n-1}}\left[\frac{(x-a)}{(x-a)^2+\varepsilon^2}\right]\right\}. \tag{2.4}$$

Note that Eq. (2.4) reduces to Eq. (2.3) for $n = 1$. For a simple pole, one also has the well-known relations[44]

$$\frac{1}{x-a\pm i\varepsilon} = \mathcal{P}\left(\frac{1}{x-a}\right) \mp i\pi\delta(x-a), \tag{2.5}$$

with the limit $\varepsilon \to 0$ on the left-hand side understood and with $\delta(x-a)$, the delta function, given by

$$\delta(x-a) = \frac{1}{\pi}\lim_{\varepsilon\to 0^+}\frac{\varepsilon}{(x-a)^2+\varepsilon^2}. \tag{2.6}$$

We emphasize again that each of the expressions in Eqs. (2.3)–(2.6) occurs in an integrand involving a single integration variable, and the range of integration can be finite or infinite.

From Eq. (2.3) one can show that[11,44]

$$\begin{aligned}\mathcal{P}\int_b^c \frac{g(x)}{(x-a)}dx &= \int_b^c \frac{\mathcal{P}}{(x-a)}g(x)dx \\ &= \lim_{\varepsilon\to 0^+}\left[\int_b^{a-\varepsilon} + \int_{a+\varepsilon}^c\right]\frac{g(x)}{(x-a)}dx,\end{aligned} \tag{2.7}$$

and if a lies outside of the range of integration $[b, c]$, then the PV integral in Eq. (2.7) becomes an ordinary integral. The limits b and c can either be finite or infinite.

Formula (2.7) shows that $\mathcal{P}$ can be written either inside or outside the integral sign. For $n > 1$, Eq. (2.4) in an integrand can be expressed as[15]

$$\mathcal{P}\int_b^c \frac{g(x)}{(x-a)^n}dx = \frac{(-)^n}{(n-1)!}\sum_{j=1}^{n-1}(-)^j\left[\Phi_j^{(a)}(c) - \Phi_j^{(a)}(b)\right] + \frac{1}{(n-1)!}\mathcal{P}\int_b^c \frac{dx}{(x-a)}\left[\frac{d^{(n-1)}}{dx^{(n-1)}}g(x)\right], \tag{2.8}$$

where

$$\begin{aligned}\Phi_j^{(a)}(u) &= \left[\frac{d^{(j-1)}}{dx^{(j-1)}}g(x)\left\{\lim_{\varepsilon\to 0+}\frac{d^{(n-1-j)}}{dx^{(n-1-j)}}\left[\frac{x-a}{(x-a)^2+\varepsilon^2}\right]\right\}\right]_{x=u}\\ &= \left[\frac{d^{(j-1)}}{dx^{(j-1)}}g(x)\ \frac{d^{(n-1-j)}}{dx^{(n-1-j)}}\left(\frac{1}{x-a}\right)\right]_{x=u},\end{aligned} \tag{2.9}$$

where the last line follows if $u \neq a$. Equation (2.8) is derived by a series of integrations by parts[15] and we obtain from Eq. (2.7)

$$\mathcal{P}\int_b^c \frac{g(x)}{(x-a)^n}dx = \frac{(-)^n}{(n-1)!}\sum_{j=1}^{n-1}(-)^j\left[\Phi_j^{(a)}(c) - \Phi_j^{(a)}(b)\right] + \frac{1}{(n-1)!}\lim_{\varepsilon\to 0}\left[\int_b^{a-\varepsilon} + \int_{a+\varepsilon}^c\right]\frac{dx}{(x-a)}\frac{d^{(n-1)}}{dx^{(n-1)}}g(x). \tag{2.10}$$

Thus we have reduced the higher-order PV integral to a simple PV expression. Invariably, this is the technique used to evaluate all higher-order PV integrals.[11,12,15] Also, in many cases the boundary terms in Eq. (2.10) vanish. We also note that

$$\frac{d^{(k)}}{dx^{(k)}}\frac{1}{(x-a)} = (-1)^k(k!)\frac{1}{(x-a)^{k+1}}, \tag{2.11}$$

so that Eq. (2.9) becomes

$$\Phi_j^{(a)}(u) = \left[\frac{(-1)^{n-1-j}(n-1-j)!}{(x-a)^{n-j}}\ \frac{d^{(j-1)}}{dx^{(j-1)}}g(x)\right]_{x=u}. \tag{2.12}$$

Thus in Eqs. (2.7) and (2.10) we have the equations for simple and higher-order pole PV integrals, respectively. In fact, we can consider Eq. (2.7) as a special case of Eq. (2.10) since, for $n = 1$, the boundary terms in Eq. (2.10) do not occur. There are two special cases of interest which we shall now consider.

2.1.2. *Infinite-limit integrals and the connection with complex variable theory*

We let $b \to -\infty$ and $c \to +\infty$ in Eq. (2.10). We also assume that the boundary terms all vanish, i.e.

$$\Phi_j(\pm\infty) = 0, \tag{2.13}$$

and that $g(x) \to g(z)$(with $z = x + iy$) is an analytic function in the upper-half plane. Then, by the standard techniques of complex variable theory[11,47], Eq. (2.10) can be expressed as

$$\mathcal{P}\int_{-\infty}^{\infty} \frac{g(x)}{(x-a)^n}dx = \frac{\pi i}{(n-1)!}\left[\frac{d^{n-1)}}{dx^{(n-1)}}g(x)\right]_{x=a}, \tag{2.14a}$$

where a is assumed to be real. If $g(z)$ is analytic in the lower-half plane, we have

$$\mathcal{P}\int_{-\infty}^{\infty} \frac{g(x)}{(x-a)^n}dx = \frac{-\pi i}{(n-1)!}\left[\frac{d^{(n-1)}}{dx^{(n-1)}}g(x)\right]_{x=a}. \tag{2.14b}$$

Equations (2.14) are the usual expressions one gets for a pole, with the PV integral differing from the usual residue expression[11,47] by the fraction, 1/2. For a simple pole, we have the important expression

$$h(a) = \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} \frac{g(x)}{(x-a)}dx, \tag{2.15}$$

which is the Hilbert transform of $g(x)$.

However, we should mention that there exist infinite-limit integrals, which one cannot easily evaluate using complex variable theory. An excellent example of such an integral is the Hilbert transform of a Gaussian, namely[2]

$$h(a) = \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} \frac{e^{-x^2}}{(x-a)}dx, \tag{2.16}$$

and e^{-z^2} is well behaved along the entire real axis, but has nontrivial analytic behavior in other parts of the complex plane. However, by a standard manipulation of this integral,[2] it can be shown that

$$h(a) = -e^{-a^2}\frac{2}{\sqrt{\pi}}\int_0^a e^{t^2}dt, \tag{2.17}$$

the right-hand side of which can be expressed in terms of the error function of imaginary argument. We emphasize that Eq. (2.17) can be derived without any assumptions on the analytic behavior of e^{-z^2}.

Consequently, we see that the complex variable theory definitions of the PV[11,47] are not the most general or even necessarily the most useful. For many cases of interest, one can easily evaluate infinite-limit, PV integrals using complex variable techniques. Such methods are particularly useful if the function $g(z)$ can be simply separated into a function which is analytic in the upper-half plane and another which is analytic in the lower-half plane. When such a separation is not possible, other methods may have to be adopted to evaluate the integral.[2] (For example, see Ref. 39.)

Also, we now see again the motivation for the $(n-1)$th derivative in Eq. (2.4). Basically, the derivative in the PV is converted to a derivative on the well-behaved function $g(x)$ by a series of integrations by parts, giving us the general expression, Eq. (2.10), which involves only a simple pole PV integral. However, the PV of a higher-order pole is automatically obtained from complex variable theory,[11,47] in which the natural definition of a residue is the $(n-1)$th derivative of $g(z)$ evaluated at the pole. If the pole is along the real axis, we get the PV, with a factor of 1/2 times the "usual" residue,[11,47] as in Eqs. (2.14). (The usual residue is for a pole entirely *within* the *closed* contour, *not* on its boundary.)

2.1.3. *Finite-limit integrals and quadrature relations*

In Eq. (2.8) we now specialize to the case in which b and c are finite. Consider the indefinite integral of the left-hand side of Eq. (2.8), namely

$$F_a(x) = \int \frac{g(x)}{(x-a)^n} dx\,. \tag{2.18}$$

The function $F_a(x)$ is then a "quadrature" of the integral. If $g(x)$ is sufficiently simple, $F_a(x)$ can usually be expressed in "closed form". However, from the fundamental theorem of integral calculus,[4] $F_a(x)$ always exists in principle.

If we perform a series of integrations by parts on the right-hand side of Eq. (2.18), we obtain[15]

$$\begin{aligned} F_a(x) = \frac{(-)^n}{(n-1)!} \sum_{j=1}^{n-1} (-1)^j \left[\frac{d^{(j-1)}}{dx^{(j-1)}} g(x)\right] \left[\frac{d^{(n-1-j)}(\frac{1}{x-a})}{dx^{(n-1-j)}}\right] \\ + \frac{1}{(n-1)!} \int \frac{dx}{(x-a)} \left[\frac{d^{(n-1)}}{dx^{(n-1)}} g(x)\right]\,. \end{aligned} \tag{2.19}$$

Equations (2.9), (2.10) and (2.19) *suggest* the following relation

$$\mathcal{P} \int_b^c \frac{g(x)}{(x-a)^n} dx = F_a(c) - F_a(b)\,, \tag{2.20}$$

so that PV is simply the *difference* of the *quadratures*. In Ref. 15, Eq. (2.20) is rigorously derived *for both* simple and higher-order poles.

Also, Eq. (2.20) shows that the PV is obtained by ignoring the singularity, i.e. "blindly integrating through the pole". As we will show more formally in the next subsection, this is because the PV is really the convergent part of the integral. Thus the next subsection is basically the *rigorous justification* of the derivation of Eq. (2.20).

There are a number of simple PV integrals that can be readily evaluated by quadratures, e.g.[15]

$$\mathcal{P} \int_b^c \frac{dx}{x} = \ln\left|\frac{c}{b}\right|, \tag{2.21a}$$

$$\mathcal{P}\int_b^c \frac{dx}{x^2} = -\frac{1}{c} + \frac{1}{b}, \tag{2.21b}$$

$$\mathcal{P}\int_b^c \frac{dx}{x^3} = -\frac{1}{2c^2} + \frac{1}{2b^2}. \tag{2.21c}$$

Also, it is sometimes convenient to shift the pole in Eq. (2.20) to the origin,[15] i.e.

$$F_a(c) - F_a(b) = \mathcal{P}\int_{b-a}^{c-a} \frac{g_a(x)}{x^n} dx, \tag{2.22}$$

where

$$g_a(x) = g(x+a). \tag{2.23}$$

2.1.4. *The PV as the convergent part of a divergent integral*

Consider a general integral of the form

$$I_a(b,c) = \sum_{j=1}^{n} \int_b^c dx \frac{g_j^{(a)}(x)}{(x-a)^n}, \tag{2.24}$$

where n refers to the *highest-order pole* in the integrand. (Also, b and/or c can be finite or infinite.) Note that $g_j^{(a)}(x)$ may contain additional powers of $(x-a)$, e.g.

$$\int_b^c dx \left[\frac{e^{-\alpha x}}{(x-a)} + \frac{e^{-\gamma x}}{(x-a)^2}\right] = \int_b^c \frac{dx}{(x-a)^2}\left[e^{-\alpha x}(x-a) + e^{-\gamma x}\right],$$

so that $g_1^{(a)}(x) = e^{-\alpha x}(x-a)$ and $g_2^{(a)}(x) = c^{-\gamma x}$.

Now in Eq. (2.24) we can expand each $g_j^a(x)$ in a Taylor series, namely

$$\begin{aligned} g_j^{(a)}(x) &= g_j^{(a)}(a) + (x-a)\left[\frac{dg_j^a(x)}{dx}\right]_{x=a} + \cdots \\ &= \sum_{k=0}^{\infty} (k!)^{-1}(x-a)^k \left[\frac{d^k}{dx^{(k)}} g_j^{(a)}(x)\right]_{x=a}. \end{aligned} \tag{2.25}$$

Then, a *sufficient condition* for the convergence of the integral $I_a(b,c)$ is the following

$$\sum_{j=1}^{n} \left[\frac{d^k}{dx^{(k)}} g_j^{(a)}(x)\right]_{x=a} = 0;\ k = 0, 1, \ldots, n-1. \tag{2.26}$$

However, note that each *separate term* in the expansion on the right-hand side of Eq. (2.24) is divergent.

Moreover, from Eq. (2.11) we see that

$$I_a(b,c) = \frac{(-)^{n-1}}{(n-1)!}\int_b^c dx \frac{d^{(n-1)}}{dx^{(n-1)}}\left(\frac{1}{x-a}\right)\sum_{j=1}^{N} g_j^{(a)}(x)\,. \tag{2.27}$$

If Eqs. (2.26) are satisfied, we can integrate by parts $n-1$ times the right-hand side of Eq. (2.27) to obtain

$$I_a(b,c) = \frac{(-1)^{n-1}}{(n-1)!}\sum_{j=1}^{N}\sum_{k=1}^{n-1}(-)^k\left[\frac{d^{(k-1)}}{dx^{(k-1)}}g_j^{(a)}(x) \times \frac{d^{(n-1-k)}}{dx^{(n-1-k)}}\frac{1}{(x-a)}\right]_{x=b}^{x=c}$$
$$+ \frac{1}{(n-1)^1}\sum_{j=1}^{N}\int_b^c \frac{dx}{(x-a)}\frac{d^{(n-1)}}{dx^{(n-1)}}g_j^{(a)}(x)\,. \tag{2.28}$$

Since $I_a(b,c)$ converges, there is no loss of generality in taking the PV of the right-hand side of Eq. (2.28), so that

$$I_a(b,c) = \frac{(-)^n}{(n-1)!}\sum_{j=1}^{N}\sum_{k=1}^{n-1}(-)^k$$
$$\times\left[\frac{d^{(k-1)}}{dx^{(k-1)}}g_j^{(a)}(x)\frac{d^{(n-1-k)}}{dx^{(n-1-k)}}\left(\frac{1}{x-a}\right)\right]_{x=b}^{x=c}$$
$$+ \frac{1}{(n-1)!}\sum_{j=1}^{N}\mathcal{P}\int_b^c \frac{dx}{(x-a)}\frac{d^{(n-1)}}{dx^{(n-1)}}g_j^{(a)}(x)\,. \tag{2.29}$$

Then, from Eqs. (2.9) and (2.10) we find

$$I_a(b,c) = \sum_{j=1}^{N}\mathcal{P}\int_b^c \frac{dx}{(x-a)^n}g_j^{(a)}(x)\,. \tag{2.30}$$

We thus obtain the important result that a convergent integral, consisting of terms each of which is separately divergent, can be evaluated by summing the PVs of each of its terms.[11,15] Thus, the PV can be interpreted as the convergent part of the integral.

We also assume that if the limits $|b|$ and $|c|$ are infinite, the appropriate boundary terms in Eq. (2.29) will vanish. There are many examples of both finite-limit and infinite-limit integrals that can be readily evaluated using Eq. (2.30) (e.g. Refs. 11 and 15)

$$I_a(b,c) = \int_b^c dx\left[\frac{R(x)}{x^2} - \frac{|\delta|}{x^2} - \frac{\gamma}{2|\delta|}\frac{1}{x}\right], \tag{2.31}$$

where δ and α are constants and

$$R(x) = \left[x^2 + \gamma x + \delta^2\right]^{1/2}\,. \tag{2.32}$$

The entire integral converges since Eq. (2.26) is satisfied, but each of the three terms on the right-hand side of Eq. (2.31) separately diverges. Also the range of integration is assumed to exclude the zeros of $R(x)$. It can then be shown that[15]

$$I(b,c) = \left[-\frac{R(x)}{x} + \ln|2R(x) + 2x + \gamma| - \frac{\gamma}{2|\delta|}\ln\left|\frac{2|\delta|R(x) + 2\delta^2 + \gamma x}{x}\right| \right.$$
$$\left. + \frac{|\delta|}{x} - \frac{\gamma}{2|\delta|}\ln|x|\right]_{x=b}^{x=c}. \tag{2.33}$$

For infinite limit integrals ($b \to -\infty, c \to +\infty$), an additional rearrangement of the integrand is desirable, namely separations into terms that are convergent in the upper- and lower-half planes. Then Eqs. (2.14) can be used to evaluate the various terms making up the integral, e.g.

$$\begin{aligned}
\int_0^\infty \left(\frac{\sin x - x\cos x}{x^3}\right) dx &= \frac{1}{2}\int_{-\infty}^\infty \left(\frac{\sin x - x\cos x}{x^3}\right) dx \\
&= \frac{1}{4}\int_{-\infty}^\infty \left[\left(\frac{e^{ix} - e^{-ix}}{ix^3}\right) - x\frac{(e^{ix} + e^{-ix})}{x^3}\right] dx \\
&= \frac{1}{4}\mathcal{P}\int_{-\infty}^\infty dx\left[-e^{ix}\left(\frac{i}{x^3} + \frac{1}{x^2}\right)\right] + \frac{1}{4}\mathcal{P}\int_{-\infty}^\infty dx\left[e^{-ix}\left(\frac{i}{x^3} - \frac{1}{x^2}\right)\right] \\
&= \frac{\pi}{4}.
\end{aligned} \tag{2.34}$$

Each term in integrand of the first line of Eq. (2.34) has a pole of order 2, but it is clear that this singularity disappears when the two terms are combined. Note too that, after we make the separation into terms proportional to e^{+ix} and e^{-ix} (which are analytic in the upper- and lower-half planes, respectively), there appear terms having poles of order 3. However, each of the final four terms may be easily evaluated using Eqs. (2.14), giving the final result.

We also remark that the material presented in this section is almost intuitively obvious to most physicists and applied mathematicians. In fact, most scientists instinctively use the approach outlined here when evaluating a convergent integral consisting of a sum of separately divergent integrals. However, a formal derivation of this method seems to be missing from the standard literature, and the justification is particularly important for cases in which one encounters higher-order poles.

Also, related discussions can be found in the mathematics literature concerning the rigorous theory of generalized functions[24,37] and of Hadamard finite-part integrals.[17] However, the language is different, and the application in generalized function theory (which is usually expressed in terms of "regularization" of divergent integrals) may not be entirely equivalent to our approach.

In Appendix A we summarize all of the many methods (see Refs. 17, 13, 15, 29, 54, 55 and 60) that have been developed for numerically evaluating PV integrals.

In all such numerical methods, we make use of the property that the PV is the convergence part of the integral. By a subtraction method, we explicitly eliminate the singularity in the integral, so that the convergent PV part can be readily evaluated.

2.2. *Formulas for multiple integrals; the Poincaré–Bertrand theorem and its generalizations*

2.2.1. *Simple poles in double integrals*

There are many examples where *two* PVs occur in a *double* integral (see Refs. 12, 15, 35, 52 and 60). In manipulating such integrals, one must be careful about *reversing the order of integration.* In particular, the PB theorem[2,12,48,57] states the following:

$$\begin{aligned}&\int_{-\infty}^{\infty} dx \frac{\mathcal{P}}{(x-u)} \int_{-\infty}^{\infty} dy \frac{\mathcal{P}}{(y-x)} f(x,y)\\&\quad= \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dx \frac{\mathcal{P}}{(x-u)} \frac{\mathcal{P}}{(y-x)} f(x,y) - \pi^2 f(u,u)\,,\end{aligned} \tag{2.35}$$

where $f(x,y)$ is well-behaved on the real axis. The last term on the right-hand side of Eq. (2.35) is the result of reversing the order of integration.

This theorem is also valid for finite-limit integrals[15,48,57], e.g.

$$\begin{aligned}&\int_{b}^{c} dx \frac{\mathcal{P}}{(x-u)} \int_{b}^{c} dy \frac{\mathcal{P}}{(yx)} f(x,y)\\&\quad= \int_{b}^{c} dy \int_{b}^{c} dx \frac{\mathcal{P}}{(x-u)} \frac{\mathcal{P}}{(y-x)} f(x,y)\\&\qquad -\pi^2 f(u,u)\Big[\Theta(c-u)\Theta(u-b) + \Theta(u-c)\Theta(b-u)\Big]\,,\end{aligned} \tag{2.36}$$

and $\Theta(\omega)$ is the Heaviside step function

$$\Theta(\omega) = \begin{cases} 1 & \text{if } \omega \geq 0 \\ 0 & \text{if } \omega < 0\,. \end{cases} \tag{2.37}$$

The limits of integration b and c are constants, independent of x and y. The final term involving the step functions in Eq. (2.36) assures us that $x = u$ or $y = u$ lie within the ranges of integration. If u is outside the ranges of integration, then both PVs become ordinary integrals, and the order of integration can be reversed without the need of the extra term. Other finite-limit expressions, analogous to Eq. (2.36), can easily be constructed (e.g., for the case in which the x and y limits are different). In Ref. 15 an example of a finite-limit, double PV integral is presented. In particular, it is shown analytically that the last term in Eq. (2.36) disappears if the range of integration does not include u. Other demonstrations of the theorem for finite-limit integrals can be performed[15] in numerical evaluations. (See Appendix A of this paper.) The derivation[11,44] showing the equivalence between Eqs. (2.3) and (2.7)

(thereby verifying the validity of interchanging the PV operation and the integral symbol) can be extended to the double integrals in Eqs. (2.35) and (2.36).

The *general rule* that one must remember in reversing the order of integration in a double integral involving two PVs is that *if one or both of the PVs disappears, the extra term does not occur.* The elimination of a PV may occur due to the limits of integration, as we have seen in Eq. (2.36). However, a PV can also be eliminated if $f(x,y)$ in Eqs. (2.35) and (2.36) is proportional to factors of $(x-u)^n, (y-u)^n$ or $(x-y)^n$ (with n a positive integer ≥ 1). In what follows we will always assume that both PVs are present in the double integral.

There are two useful identities that occur in this formalism. First, we have[12,48]

$$\frac{\mathcal{P}}{(x-u)}\frac{\mathcal{P}}{(y-x)} = \frac{\mathcal{P}}{(y-u)}\left[\frac{\mathcal{P}}{(x-u)} - \frac{\mathcal{P}}{(x-y)}\right]. \tag{2.38}$$

Equation (2.38) can formally be justified using the fundamental PV definition, Eq. (2.3) and then taking a limiting procedure. However, Eq. (2.38) is almost obvious. Clearly, it is valid if there are no PVs present (i.e. if $x \neq u, y \neq u$, and $y \neq x$). Recall from Sec. 2.2 that, when one takes a PV, one is eliminating the divergence due to the pole. Thus, basically Eq. (2.38) is valid because of the "regularization" property inherent in all PV expressions.[24,37]

The second important identity is a generalization of the familiar Eq. (2.5). If there are two poles present in an integrand, one can show that,[12,49]

$$\begin{aligned}\left[(x-u_1-is_1\varepsilon_1)(x-u_2-is_2\varepsilon_2)\right]^{-1} \underset{\varepsilon_1,\varepsilon_2\to 0}{\longrightarrow} \left[\frac{\mathcal{P}}{x-u_2} + i\pi s_1\delta(x-u_1)\right] \\ \times\left[\frac{\mathcal{P}}{x-u_2} + i\pi s_2\delta(x-u_2)\right] + \pi^2\delta(x-u_1)\delta(x-u_2)\,,\end{aligned} \tag{2.39}$$

where $s_i = \pm 1$. The last term in Eq. (2.39) arises from the last (extra) term present in the PB expressions (2.35) and (2.36). It is clear that in using Eq. (2.39) in an integral, a PV must not be eliminated for any reason; e.g., the range of integration must include both u_1 and u_2.

Examples of the usefulness of the PB will be discussed in Secs. 4–6. However, there is a simple mathematical example which we now present. Let $h(x)$ be the Hilbert transform of $g(x)$. Then, from Eq. (2.15) we have

$$h(x) = \frac{1}{\pi}\int_{-\infty}^{\infty} dy \frac{\mathcal{P}}{y-x} g(y)\,. \tag{2.40}$$

Next, construct the function

$$\begin{aligned}\hat{g}(u) &= \frac{1}{\pi}\int_{-\infty}^{\infty} dx \frac{\mathcal{P}}{x-u} h(x) \\ &= \frac{1}{\pi^2}\int_{-\infty}^{\infty} dx \frac{\mathcal{P}}{x-u}\int_{-\infty}^{\infty} dy \frac{\mathcal{P}}{y-x} g(y),\end{aligned} \tag{2.41}$$

which from Eq. (2.35) becomes

$$\hat{g}(u) = \frac{1}{\pi^2}\int_{-\infty}^{\infty} g(y)dy \int_{-\infty}^{\infty} dx \frac{\mathcal{P}}{(x-u)}\frac{\mathcal{P}}{(y-x)} - g(u)\,. \tag{2.42}$$

It can be shown that

$$\int_{-\infty}^{\infty} dx \frac{\mathcal{P}}{(x-u)}\frac{\mathcal{P}}{(y-x)} = 0 \ (u \text{ real})\,, \tag{2.43}$$

whereby Eq. (2.42) becomes

$$\hat{g}(u) = -g(u) = \frac{1}{\pi}\int_{-\infty}^{\infty} dx \frac{\mathcal{P}}{x-u} h(x)\,. \tag{2.44}$$

Thus, we obtain the well-known result[1,22,47] that if h is the Hilbert transform of g, then g is (minus) the Hilbert transform of h. This result is usually proven by complex variable theory by letting $z \to x + iy$ and requiring that $\psi^{(+)}(z) = h(z) + ig(z)$ be an analytic function in the upper-half plane. Here the result has been established without any assumptions on analyticity. Nevertheless, we know from a fundamental theorem due to Titchmarsh[56] that there is an intimate connection between analyticity and the existence of Hilbert transforms. We shall discuss Titchmarsh's theorem in much more detail in Sec. 3.

2.2.2. *Higher-order poles in double integrals*

The PB theorem can also be generalized to higher-order poles. It has been shown that[12]

$$\begin{aligned}
&\int_{-\infty}^{\infty} dx \frac{\mathcal{P}}{(x-u)^n}\int_{-\infty}^{\infty} dy \frac{\mathcal{P}}{(y-x)^m} f(x,y) \\
&\quad = \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dx \frac{\mathcal{P}}{(x-u)^n}\frac{\mathcal{P}}{(y-x)^m} f(x,y) \\
&\qquad - \frac{\pi^2}{(n-1)!(m-1)!}\sum_{r=0}^{n-1}\binom{n-1}{r}\left[\frac{\partial^{(n-1-r)}}{\partial x^{(n-1-r)}}\frac{\partial^{(m-1+r)}}{\partial y^{(m-1+r)}} f(x,y)\right]_{x=y=u},
\end{aligned} \tag{2.45}$$

where

$$\binom{N}{r} = \frac{N!}{r!(N-r)!}\,. \tag{2.46}$$

Note that Eq. (2.45) reduces to Eq. (2.35) for $n = m = 1$, for which the only contribution to the sum on the right-hand side of Eq. (2.45) is for $r = 0$.

In the derivation[12] of Eq. (2.45), the following partial fraction expression was used

$$
\begin{aligned}
\frac{\mathcal{P}}{(x-u)^n}\frac{\mathcal{P}}{(x-y)^m} = {} & \frac{(-)^m}{(m-1)!}\sum_{r=0}^{n-1}\frac{(m+r-1)!}{r!} \\
& \times \left[\frac{\mathcal{P}}{(x-u)^{n-r}}\frac{\mathcal{P}}{(y-u)^{m+r}}\right. \\
& + (-)^{m+r}\left[(n-1-r)!\right]^{-1}\sum_{r'=0}^{m+r-1}(-)^{r'}\frac{(n+m-r'-2)!}{(m+r-1-r')!} \\
& \left.\times \frac{\mathcal{P}}{(y-u)^{r'+1}}\frac{\mathcal{P}}{(x-y)^{m+n-r'-1}}\right]. \qquad (2.47)
\end{aligned}
$$

However, it is clear that the left-hand side of Eq. (2.47) is invariant under the interchange of u and y *and* of n and m. Thus, we find that[14]

$$
\begin{aligned}
\frac{\mathcal{P}}{(x-u)^n}\frac{\mathcal{P}}{(x-y)^m} = {} & \frac{(-)^n}{(n-1)!}\sum_{r=0}^{m-1}\frac{(n+r-1)!}{r!} \\
& \times \left[\frac{\mathcal{P}}{(x-y)^{m-r}}\frac{\mathcal{P}}{(u-y)^{n+r}}\right. \\
& + (-)^{n+r}\left[(m-1-r)!\right]^{-1}\sum_{r'=0}^{n+r-1}(-)^{r'}\frac{(m+n-r'-2)!}{(n+r-1-r')!} \\
& \left.\times \frac{\mathcal{P}}{(u-y)^{r'+1}}\frac{\mathcal{P}}{(x-u)^{m+n-r'-1}}\right]. \qquad (2.48)
\end{aligned}
$$

However, because of the symmetry of the left-hand side of Eq. (2.47), yet a third (manifestly symmetric) expression can be derived,[14] namely

$$
\begin{aligned}
\frac{\mathcal{P}}{(x-u)^m}\frac{\mathcal{P}}{(x-y)^m} = {} & \frac{(-)^m}{(m-1)!}\sum_{r=0}^{n-1}\frac{(m+r-1)!}{r!}\frac{\mathcal{P}}{(x-u)^{n-r}}\frac{\mathcal{P}}{(y-u)^{m+r}} \\
& + \frac{(-)^n}{(n-1)!}\sum_{r=0}^{m-1}\frac{(n+r-1)!}{r!}\frac{\mathcal{P}}{(x-y)^{m-r}}\frac{\mathcal{P}}{(u-y)^{n+r}}. \qquad (2.49)
\end{aligned}
$$

Note the high degree of symmetry present in Eq. (2.49) as compared to Eqs. (2.47) and (2.48). All three expressions are equivalent[14] and can be used to derive variations of the PB theorem for higher-order poles. Also, the remarks regarding the derivation and validity of Eq. (2.38) also apply to Eqs. (2.47), (2.48) and (2.49).

2.2.3. *Simple poles in general multiple integrals*

The final generalization of the PB theory is for multiple PV integrals which contain only simple poles.[12] We define the following functions:

$$\mathcal{A}_n^{(f)}(u) = \int \frac{\mathcal{P}}{(x_1 - u)} dx \int \frac{\mathcal{P}}{(x_2 - x_1)} dx_2 \int \frac{\mathcal{P}}{(x_3 - x_2)} dx_3 \times \cdots \times \int \frac{\mathcal{P}}{(x_n - x_1)} dx_n \, f_n(x_1, x_2, x_3, \ldots, x_n) \tag{2.50}$$

and

$$\mathcal{B}_n^{(f)}(u) = \int dx_n \int dx_{n-1} \cdots \int dx_2 \int dx_1 \times \frac{\mathcal{P}}{(x_1 - u)} \frac{\mathcal{P}}{(x_n - x_1)} f_n(x_1, x_2, \cdots, x_n), \tag{2.51}$$

and for simplicity of notation we do not put the limits on the integrals since the formulas that we present pertain either to finite-limit or to infinite-limit integrations. (As in Subsec. 2.2.1, it is assumed that no PV is removed in any of the integrals.) The function $f_n(x_1, x_2, \ldots, x_n)$ is assumed to be well-behaved over all of the n domains of integration.

By comparing the definitions in Eqs. (2.50) and (2.51) with Eq. (2.35), it is clear that the natural generation of the PB theorem to multiple integrals can be expressed as

$$\mathcal{A}_n^{(f)}(u) = \mathcal{B}_n^{(f)}(u) + \mathcal{D}_n^{(f)}(u), \tag{2.52}$$

where $\mathcal{D}_n^{(f)}(u)$ is the extra term resulting from exchanging the various orders of integration in going from $\mathcal{A}_n^{(f)}(u)$ to $\mathcal{B}_n^{(f)}(u)$. Of course, for $n = 2$ we have from Eq. (2.35)

$$\mathcal{D}_2^{(f)}(u) = -\pi^2 f_2(u, u), \tag{2.53}$$

and, after extensive manipulations, one finds that[12]

$$\mathcal{D}_3^{(f)}(u) = \pi^2 \int \frac{\mathcal{P}}{(x - u)} dx \left[f_3(x, x, x) - f_3(u, x, u) - f_3(u, u, x) \right]. \tag{2.54}$$

Now, a general expression for $\mathcal{D}_n^{(f)}(u)$ can be written but it is rather unwieldy and not very useful. Therefore, we shall instead give a rather practical recursion relation for finding $\mathcal{D}_n^{(f)}(u)$ for relatively small values of n (say, $n \leq 5$).

Suppose that we have a function of $n + 1$ variables, namely

$$f_{n+1}(x_1, x_2, \ldots, x_n, x_{n+1}),$$

and we eliminate the last variable by *defining* another function

$$g_n(x_1, x_r, \ldots, x_n) = \int \frac{\mathcal{P}}{(x_{n+1} - x_n)} dx_{n+1} f_{n+1}(x_1, x_2, \ldots, x_n, x_{n+1}). \tag{2.55}$$

Now assume that $\mathcal{D}_n^{(g)}(u)$ is known for $g_n(x_1, x_2, \ldots, x_n)$. Then, it can be shown that[12]

$$\mathcal{D}_{n+1}^{(f)}(u) = \mathcal{D}_n^{(g)}(u) + (-)^n \pi^2 \int dx_n \int dx_{n-1} \cdots \int dx_2$$
$$\times \left[\frac{\mathcal{P}}{\prod_{j=2}^{n}(u - x_j)} f_{n+1}(u, x_2, x_3, \ldots, x_n, u) \right.$$
$$\left. + \sum_{i=2}^{n} \frac{\mathcal{P}}{(x_i - u)\prod_{\substack{j=2\\ j\neq i}}^{n}(x_i - x_j)} f_{n+1}(x_i, x_2, \ldots, x_n, x_i) \right] . \quad (2.56)$$

We note that in the last two lines of Eq. (2.56) the first and last variable positions in f_{n+1} are taken up, first, by u and then by x_1. Also, we do not integrate over either x_1 or x_{n+1}. This asymmetry in coordinates results from the special link between x_1 and x_n in Eqs. (2.50) and (2.51). As an example, consider a function $f_3(x, y, z)$ for which we define

$$g_2(x, y) = \int \frac{\mathcal{P}}{z - y} dz f_3(x, y, z) , \quad (2.57)$$

and from Eq. (2.56) we find that

$$\mathcal{D}_3^{(f)}(u) = \mathcal{D}_2^{(g)}(u) + \pi^2 \int dy \left[\frac{\mathcal{P}}{u - y} f(u, y, u) + \frac{\mathcal{P}}{y - u} f(y, y, y) \right] . \quad (2.58)$$

From Eqs. (2.53) and (2.57), this becomes

$$\mathcal{D}_3^{(f)}(u) = -\pi^2 \int \frac{\mathcal{P}}{z - u} dz f_3(u, u, z)$$
$$+ \pi^2 \int dy \left[\frac{\mathcal{P}}{u - y} f(u, y, u) + \frac{\mathcal{P}}{y - u} f(y, y, y) \right] , \quad (2.59)$$

which is Eq. (2.54). Then, since we have the general structure of $\mathcal{D}_3^{(f)}(u)$, we can find $\mathcal{D}_4^{(f)}(u)$ and higher-order $\mathcal{D}_n^{(f)}$ functions. Of course, in practice one is limited to rather small values of n (say, $n \leq 5$); otherwise, Eq. (2.56) becomes very difficult to use. Note also that the asymmetry in the coordinate positions in Eq. (2.54), again resulting from the asymmetry inherent in the original equations (2.50) and (2.51).

We remark too that the $\mathcal{P}$'s appearing in the second and third lines of Eq. (2.56) have the following meaning[12]

$$\frac{\mathcal{P}}{\prod_{i=1}^{n}(x - x_i)} = \sum_{j=1}^{n} \frac{\mathcal{P}}{(x - x_i)} K_i^{(n)} , \quad (2.60)$$

where

$$K_i^{(n)} = \left[\prod_{\substack{j=1\\ j\neq i}}^{n} (x_i - x_j) \right]^{-1} . \quad (2.61)$$

Thus, a PV involving a product of factors can be expressed as a sum of the PVs of each of the individual functions. These remarks, coupled with the results in

Eqs. (2.47)–(2.49) imply that we can always express a complicated PV (involving a product containing poles of arbitrary order) in a partial fraction expression. In fact, a general expansion for a PV of the form

$$\frac{\mathcal{P}}{\prod_{i=1}^{N}(x-t_i)^{n_i}} \qquad (N, n_i \geq 1)$$

is given in Ref. 14. In this case, the expansion is in terms of individual *higher-order* PVs such as

$$\frac{\mathcal{P}}{(x-t_i)^{m_i}} \qquad (m_i \geq 1)\,.$$

Equation (2.60) yields another interesting identity. It is well known that

$$\int_{-\infty}^{\infty} \frac{\mathcal{P}}{(x-a)} dx = 0 \qquad a \text{ real.} \tag{2.62}$$

Thus, from Eqs. (2.60) and (2.62) we find that

$$\int_{-\infty}^{\infty} \frac{\mathcal{P}}{\prod_{i=1}^{N}(x-x_i)} = 0 \qquad (x_i \text{ all real})\,. \tag{2.63}$$

One other important identity should be stated, namely

$$\mathcal{P}\int_{0}^{\infty} \frac{dx}{x^2-a^2} = 0, \tag{2.64}$$

which can be proven by a partial fraction expansion and a limiting procedure.

Finally, it should be mentioned that in Ref. 12 other generalizations of the PB theorem to multiple integrals were considered (i.e. generalizations other than (2.50)–(2.52)). It was concluded that such generalizations are difficult to construct and appear to be uninteresting and useless. On the other hand, the generalization given here has many applications, an example of which is given in Sec. 3.

3. Dispersion Relations

3.1. *Dispersion relations for advanced, retarded, and causal Green's functions*

It is very useful to have a relation between the real and imaginary parts of a Green's function. For example, in the case of a finite-temperature *causal Green's function* (or propagator), there is an important dispersion relation[23]

$$\mathrm{Re}\,[G(\omega)] = \frac{1}{\pi}\int_{-\infty}^{\infty} d\omega' \frac{\mathcal{P}}{(\omega'-\omega)} \mathrm{Im}\,[G(\omega')]\,\eta(\omega')\,, \tag{3.1}$$

where the Green's function, $G(\omega)$, is in the energy representation ($E = \hbar\omega$) and

$$\eta(\omega) = \begin{cases} \tanh\left[(\omega-\mu)/2k_{\mathrm{B}}T\right] & \text{for bosons} \\ \coth\left[(\omega-\mu)/2k_{\mathrm{B}}T\right] & \text{for fermions;} \end{cases} \tag{3.2}$$

μ is the chemical potential, k_{B} is the Boltzmann constant, and T is the temperature.

In the zero temperature limit, we have

$$\eta(\omega) \xrightarrow[T\to 0]{} \text{sign}\,(\omega-\mu)\,. \tag{3.3}$$

Then, from Eqs. (2.40) and (2.44) we find that

$$\text{Im}\,[G(\omega)]\,\eta(\omega) = -\frac{1}{\pi}\int_{-\infty}^{\infty} d\omega' \frac{\mathcal{P}}{(\omega'-\omega)}\text{Re}\,[G(\omega')]\,. \tag{3.4}$$

For the *advanced* and *retarded* Green's functions, the above formulas also apply, except for Eq. (3.2), which becomes

$$\eta(\omega) = \begin{cases} +1 & \text{for the retarded function} \\ -1 & \text{for the advanced function.} \end{cases} \tag{3.5}$$

Sometimes it is useful to resort to the time representation using the Fourier transform

$$G(t) = \int_{-\infty}^{\infty} d\omega\; e^{-i\omega t} G(\omega)\,. \tag{3.6}$$

The inverse of the Fourier transform (3.6) is

$$G(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dt\; e^{i\omega t} G(t)\,. \tag{3.7}$$

3.2. *Titchmarsh's theorem*

The theorem[56] states that, for $f_1(x)$ and $f_2(x)$ Lebesgue square integrable functions for all values of x, the following properties imply one another:

(a) $F(z) = f_1(z) + if_2(z), z = x + iy$, is an analytic function in the *upper-half plane*, with

$$\int_{-\infty}^{\infty} |\, F(z)\,|^2\, dx \text{ finite for } y > 0. \tag{3.8}$$

(b) $f_1(x)$ and $f_2(x)$ are Hilbert transform of one another, with

$$f_1(x) = \frac{\mathcal{P}}{\pi}\int_{-\infty}^{\infty} \frac{dx'}{(x'-x)} f_2(x')\,. \tag{3.9}$$

(c) The Fourier transform of $F(x)$ is proportional to a step function. Specifically, identifying x with an energy or frequency representation, $x \to \omega$, we find that in the Fourier transform (time) representation

$$F(t) = \int_{-\infty}^{\infty} d\omega\; e^{-i\omega t} F(\omega) \tag{3.10a}$$

$$= \Theta(t) G(t)\,. \tag{3.10b}$$

This last property is the causal condition. The validity of any one of these three conditions implies the other two. Thus, we see very clearly from this theorem the equivalence of the existence of a Hilbert transform, analyticity, and causality.

Also, we mention that for a function that is analytic in the *lower*-half plane, the Hilbert transform alters sign in Eq. (3.9) and Eq. (3.10b) is replaced by

$$F(t) = \Theta(-t)G(t)\,. \tag{3.11}$$

It is instructive to give a partial proof of Titchmarsh's theorem since some results of this proof will be useful in further work.[41] We do *not* attempt to establish the connection between condition (a) and conditions (b) and (c), so we make no assumption about analyticity or square integrability. However, we will demonstrate that conditions (b) and (c) imply one another.

In the proofs that follow, the reader may notice that the order of integration is reversed for double integrals containing a PV. This does not contradict the results of Sec. 2.2 since the integrals in question contain only *one* (not *two*) PV. In fact, in integrals containing products of Schwartz distributions[2] (e.g., PVs, delta functions, or step functions), the order of integrations can always be reversed provided that only one PV is present. (That is, in a double integral containing two delta functions or a delta function and a PV, the order of integrations can be freely exchanged.)

First, assume Eq. (3.10b), where $F(t)$ has the Fourier transform

$$F(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} F(t)e^{i\omega t}dt\,. \tag{3.12}$$

Next construct the function

$$I(\omega) = \frac{\mathcal{P}}{\pi}\int_{-\infty}^{\infty} \frac{\mathrm{Im}\,[F(\omega')]}{(\omega' - \omega)}d\omega', \tag{3.13}$$

which becomes

$$I(\omega) = \frac{1}{2\pi^2}\,\mathrm{Im}\left[\int_0^{\infty} G(t)dt\ \mathcal{P}\int_{-\infty}^{\infty} \frac{e^{i\omega' t}}{(\omega' - \omega)}d\omega'\right]. \tag{3.14}$$

However, from complex variable theory we know that

$$\mathcal{P}\int_{-\infty}^{\infty} \frac{e^{i\omega' t}}{(\omega' - \omega)}d\omega' = \pi i\,[\Theta(t) - \Theta(-t)]\,e^{i\omega t}, \tag{3.15}$$

which gives

$$\begin{aligned} I(\omega) &= \frac{1}{2\pi}\,\mathrm{Im}\left[i\int_0^{\infty} G(t)e^{i\omega t}dt\right] \\ &= \frac{1}{2\pi}\,\mathrm{Im}\left[i\int_{-\infty}^{\infty} F(t)e^{i\omega t}dt\right] \\ &= \mathrm{Re}\,[F(\omega)]\,, \end{aligned} \tag{3.16}$$

the desired dispersion relation. Thus, condition (c) implies condition (b).

Now *assume* the existence of the dispersion relation

$$\operatorname{Re}[F(\omega)] = \frac{\mathcal{P}}{\pi}\int_{-\infty}^{\infty} d\omega' \frac{\operatorname{Im}[F(\omega')]}{(\omega'-\omega)}, \tag{3.17}$$

so that

$$\begin{aligned} F(\omega) &= \operatorname{Re}[F(\omega)] + i\operatorname{Im}[F(\omega)] \\ &= \frac{1}{\pi}\int_{-\infty}^{\infty} d\omega' \left[\frac{\mathcal{P}}{(\omega'-\omega)} + i\pi\delta(\omega'-\omega)\right] \operatorname{Im}[F(\omega')], \end{aligned} \tag{3.18}$$

which from Eq. (2.5) becomes

$$F(\omega) = \frac{1}{\pi}\int_{-\infty}^{\infty} d\omega' \frac{\operatorname{Im}[F(\omega')]}{(\omega'-\omega-i\varepsilon)}. \tag{3.19}$$

Now, the Fourier transform of $F(\omega)$ is given by

$$F(t) = \frac{1}{\pi}\int_{-\infty}^{\infty} d\omega' \operatorname{Im}[F(\omega')] \int_{-\infty}^{\infty} \frac{e^{-i\omega t}d\omega}{(\omega'-\omega-i\varepsilon)}. \tag{3.20}$$

Then, since we have

$$\lim_{\varepsilon\to 0^+}\int_{-\infty}^{\infty} \frac{e^{-i\omega t}}{\omega'-\omega-i\varepsilon} d\omega = +2\pi i e^{-i\omega' t}\Theta(t), \tag{3.21}$$

Eq. (3.20) becomes

$$F(t) = 2i\Theta(t)\int_{-\infty}^{\infty} d\omega' e^{-i\omega' t} \operatorname{Im} F(\omega'), \tag{3.22}$$

which is proportional to the required $\Theta(t)$.

Thus, we see that the existence of a Hilbert transform implies causality, and vice versa, with no particular assumptions about the analytic properties or square integrability of $F(\omega)$. The complete proof of the theorem[56] establishes the final connections, linking analyticity, causality, and the existence of Hilbert transforms.

A useful identity also follows from Eq. (3.22) of Ref. 41. First, we note that

$$\begin{aligned} F(\omega) &= \operatorname{Re}[F(\omega)] + i\operatorname{Im}[F(\omega)] \\ &\equiv f_1(\omega) + i f_2(\omega), \end{aligned} \tag{3.23}$$

from which we obtain

$$F(t) = f_1(t) + i f_2(t). \tag{3.24}$$

Of course, $f_1(\omega)$ and $f_2(\omega)$ are real functions by definition, but $f_1(t)$ and $f_2(t)$ are clearly complex. Then, from Eqs. (3.10a) and (3.22)-(3.24), we find that[41]

$$\begin{aligned} f_1(t) &= -i f_2(t) + i2\Theta(t) f_2(t) \\ &= i f_2(t)\left[-\Theta(t) - \Theta(-t) + 2\Theta(t)\right] \end{aligned} \tag{3.25}$$

or

$$f_1(t) = i\,[\Theta(t) - \Theta(-t)]\,f_2(t) \tag{3.26}$$

or

$$f_2(t) = -i\,[\Theta(t) - \Theta(-t)]\,f_1(t)\,, \tag{3.27}$$

where we have used the identities

$$1 = \Theta(t) + \Theta(-t) \tag{3.28}$$

and

$$\Theta(t)\Theta(-t) = 0. \tag{3.29}$$

Also, from Eqs. (3.24), (3.26), (3.27) and (3.28) we obtain[41]

$$F(t) = 2i\Theta(t)f_2(t) \tag{3.30a}$$

$$= 2\Theta(t)f_1(t)\,. \tag{3.30b}$$

Thus, we see that, in either the ω or t representations, there is only one independent function (either f_1 or f_2). This behavior, of course, arises because of the existence of the Hilbert transform, Eq. (3.9). Also, as before we make no assumptions about analyticity in deriving Eqs. (3.26), (3.27), and (3.30).

3.3. *Application of the Poincaré–Bertrand theorem to response functions or two-particle loop integrals*

The response function,[23] or loop integral,[12,52,60] is proportional to the energy-representation integral

$$\Pi_{\alpha\beta}(\omega) = i\int_{-\infty}^{\infty} d\omega' G_\alpha(\omega+\omega')G_\beta(\omega')\,. \tag{3.31}$$

(See Fig. 1 for the appropriate Feynman diagram.) In Eq. (3.31) G_α and G_β are the propagators for particles α and β, respectively. In the time representation, Eq. (3.6), Eq. (3.31) becomes

$$\Pi_{\alpha\beta}(t) = iG_\alpha(t)G_\beta(-t) \tag{3.32a}$$

or

$$\Pi_{\alpha\beta}(t-t') = iG_\alpha(t-t')G_\beta(t'-t)\,, \tag{3.32b}$$

which accounts for the loop occurring in the response function.

We assume now that α and β pertain to Green's functions that satisfy the dispersion relations (3.1) and (3.4). For causal functions, $\eta_\alpha(\omega)$ and $\eta_\beta(\omega)$ are given by Eq. (3.2), while for retarded and advanced propagators we use Eq. (3.5).

Then, the imaginary part of Eq. (3.31) is given by

$$\mathrm{Im}[\Pi_{\alpha,\beta}(\omega)] = \int_{-\infty}^{\infty} d\omega' \Big\{ \mathrm{Re}\,[G_\alpha(\omega+\omega')]\,\mathrm{Re}[G_\beta(\omega')] - \mathrm{Im}[G_\alpha(\omega+\omega')]\mathrm{Im}[G_\beta(\omega')] \Big\} . \tag{3.33}$$

From Eq. (3.1), we obtain

$$\begin{aligned}\int_{-\infty}^{\infty} d\omega' \ \mathrm{Re}\,[G_\alpha(\omega+\omega')] \ \ \mathrm{Re}\,[G_\beta(\omega')] &= \frac{1}{\pi^2}\int_{-\infty}^{\infty} d\omega' \int_{-\infty}^{\infty} d\omega_\alpha \frac{\mathcal{P}}{(\omega_\alpha-\omega'-\omega)} \ \mathrm{Im}\,[G_\alpha(\omega_\alpha)] \\ &\times \eta_\alpha(\omega_\alpha) \int_{-\infty}^{\infty} d\omega_\beta \frac{\mathcal{P}}{(\omega_\beta-\omega')} \ \mathrm{Im}\,[G_\beta(\omega_\beta)]\,\eta_\beta(\omega_\beta) .\end{aligned} \tag{3.34}$$

Now, in Eq. (3.34) we can interchange the ω' and ω_α integrations since only one PV is present,[2] and from Eq. (2.35) we find that

$$\begin{aligned}\int_{-\infty}^{\infty} d\omega' \ \mathrm{Re}\,[G_\alpha(\omega+\omega')]\,\mathrm{Re}\,[G_\beta(\omega')] &= \frac{1}{\pi^2}\int_{-\infty}^{\infty} d\omega_\alpha \ \mathrm{Im}\,[G_\alpha(\omega_\alpha)]\,\eta_\alpha(\omega_\alpha)\int_{-\infty}^{\infty} d\omega_\beta \mathrm{Im}\,[G_\beta(\omega_\beta)]\,\eta_\beta(\omega_\beta) \\ &\times \int_{-\infty}^{\infty} d\omega' \frac{\mathcal{P}}{(\omega_\alpha-\omega'-\omega)}\frac{\mathcal{P}}{(\omega_\beta-\omega')} \\ &+ \int_{-\infty}^{\infty} d\omega_\alpha \ \mathrm{Im}\,[G_\alpha(\omega_\alpha)]\,\eta_\alpha(\omega_\alpha)\mathrm{Im}\,[G_\beta(\omega_\alpha-\omega)]\,\eta_\beta(\omega_\alpha-\omega) .\end{aligned} \tag{3.35}$$

From Eq. (2.63), the first term in Eq. (3.35) vanishes and after redefining variables, Eq. (3.33) becomes

$$\begin{aligned}\mathrm{Im}\,[\Pi_{\alpha\beta}(\omega)] &= \int_{-\infty}^{\infty} d\omega_\alpha \int_{-\infty}^{\infty} d\omega_\beta \ \delta(\omega_\alpha-\omega-\omega_\beta) \\ &\times \ [\eta_\alpha(\omega_\alpha)\eta_\beta(\omega_\beta)-1] \ \mathrm{Im}\,[G_\alpha(\omega_\alpha)] \ \mathrm{Im}\,[G_\beta(\omega_\beta)] .\end{aligned} \tag{3.36}$$

From Eqs. (3.1) and (3.31), we obtain

$$\begin{aligned}\mathrm{Re}\,[\Pi_{\alpha\beta}(\omega)] &= -\frac{1}{\pi}\int_{-\infty}^{\infty} d\omega_\alpha \int_{-\infty}^{\infty} d\omega_\beta \\ &\times \frac{\mathcal{P}}{(\omega_\alpha-\omega-\omega_\beta)} \ \mathrm{Im}\,[G_\alpha(\omega_\alpha)] \ \mathrm{Im}\,[G_\beta(\omega_\beta)] \\ &\times \ [\eta_\alpha(\omega_\alpha)-\eta_\beta(\omega_\beta)] ,\end{aligned} \tag{3.37}$$

and it is clear from Eqs. (3.36) and (3.37) that the following dispersion relation is valid

$$\mathrm{Re}\,[\Pi_{\alpha\beta}(\omega)] = \frac{1}{\pi}\int_{-\infty}^{\infty} d\omega' \frac{\mathcal{P}}{(\omega'-\omega)}\mathrm{Im}\,[\Pi_{\alpha\beta}(\omega')]\,\eta_{\alpha\beta}(\omega')\,, \tag{3.38}$$

where

$$\eta_{\alpha\beta}(\omega_\alpha - \omega_\beta) = \frac{\eta_\beta(\omega_\beta) - \eta_\alpha(\omega_\alpha)}{\eta_\alpha(\omega_\alpha)\eta_\beta(\omega_\beta) - 1}\,. \tag{3.39}$$

If α and β pertain to finite-temperature causal Green's functions, then from Eqs. (3.2) and (3.39) we obtain[12]

$$\eta_{\alpha\beta}(\omega) = \begin{cases} \tanh\,[(\omega - \mu_\alpha + \mu_\beta/2\kappa_B T] \\ \text{if } \alpha \text{ and } \beta \text{ are particles with like statistics}\,, \\ \coth\,[(\omega - \mu_\alpha + \mu_\beta)/2k_B T] \\ \text{if } \alpha \text{ and } \beta \text{ are particles with unlike statistics.} \end{cases} \tag{3.40}$$

This result states that if both particles are bosons or both are fermions, then the loop integral behaves as a boson. On the other hand, if one particle is a boson and the other is a fermion, the loop behaves as a fermion. In the zero-temperature limit, we have

$$\eta_{\alpha\beta}(\omega) \underset{T\to 0}{\longrightarrow} \text{sign}\;(\omega - \mu_\alpha + \mu_\beta)\,. \tag{3.41}$$

If the propagators are retarded and advanced Green's functions, we find that

$$\eta_{\alpha\beta}(\omega) = \begin{cases} 0, & \text{if both propagators are} \\ & \text{retarded or advanced functions,} \\ +1, & \text{for } \alpha \text{ retarded, } \beta \text{ advanced,} \\ -1, & \text{for } \alpha \text{ advanced, } \beta \text{ retarded.} \end{cases} \tag{3.42}$$

Equation (3.42) is a consequence of the physics which demands that, in the zero-temperature limit, only *particle-hole combinations* are allowed in the response function. In fact, this result can be seen more generally from Eqs. (3.36) and (3.37) if we take[12] $T \to 0$. In that limit, particle-particle and hole-hole contributions identically vanish. Of course, for finite temperatures, the particle-hole boundaries are *smeared*, and one *cannot* make an unambiguous identification of a particle-hole pair.

3.4. *The Poincaré–Bertrand theorem applied to three-particle loop integrals*

It is of interest to consider the generalization of the PB theorem to triple PV integrals, for which one uses Eqs. (2.50)–(2.52), for $n = 3$, and Eq. (2.54). Such analyses then give much insight into how to generalize the results to multiple integrals of arbitrary order. Two special cases of interest were treated in Ref. 12:

(i) convolutions with respect to time and (ii) triple-propagator loop integrals. In this section we will discuss only the latter.

In Fig. 2, we display the triple-propagator loop integral, which is given by

$$L_{\alpha\beta\gamma}(\omega) = \int_{-\infty}^{\infty} d\omega_\alpha \int_{-\infty}^{\infty} d\omega_\beta G_\alpha(\omega_\alpha) G_\beta(\omega_\beta) G_\gamma(\omega_\alpha + \omega_\beta + \omega) . \tag{3.43}$$

Then, from Eqs. (3.6) and (3.7), it can be shown that in the time representation we have

$$L_{\alpha\beta\gamma}(t) = G_\alpha(-t) G_\beta(-t) G_\gamma(t) , \tag{3.44}$$

and the direction of the arrows in Fig. 2 clearly correspond to the time arguments in Eq. (3.44).

From Eqs. (2.50)–(2.52), (2.54) and (3.1), we find that[12]

$$\begin{aligned} \mathrm{Re}\ [L_{\alpha\beta\gamma}(\omega)] = {} & \frac{\mathcal{P}}{\pi} \int_{-\infty}^{\infty} d\omega_\alpha \int_{-\infty}^{\infty} d\omega_\beta \int_{-\infty}^{\infty} d\omega_\gamma \\ & \times \frac{\mathrm{Im}\,[G_\alpha(\omega_\alpha)]\ \mathrm{Im}\,[G_\beta(\omega_\beta)]\ \mathrm{Im}\,[G_\gamma(\omega_\gamma)]}{(\omega + \omega_\alpha + \omega_\beta - \omega_\gamma)} \\ & \times\ [\eta_\alpha(\omega_\alpha)\eta_\beta(\omega_\beta)\eta_\gamma(\omega_\gamma) - \eta_\alpha(\omega_\alpha) - \eta_\beta(\omega_\beta) + \eta_\gamma(\omega_\gamma)] . \end{aligned} \tag{3.45}$$

Also, one can show that

$$\begin{aligned} \mathrm{Im}[L_{\alpha\beta\gamma}(\omega)] = {} & \int_{-\infty}^{\infty} d\omega_\alpha \int_{-\infty}^{\infty} d\omega_\beta \\ & \times \mathrm{Im}[G_\alpha(\omega_\alpha)]\ \mathrm{Im}[G_\beta(\omega_\beta)]\ \mathrm{Im}[G_\gamma(\omega_\alpha + \omega_\beta + \omega)] \\ & \times\ [\eta_\beta(\omega_\beta)\eta_\gamma(\omega_\alpha + \omega_\beta + \omega) + \eta_\gamma(\omega_\alpha + \omega_\beta + \omega)\eta_\alpha(\omega_\alpha) \\ & -\ \eta_\alpha(\omega_\alpha)\eta_\beta(\omega_\beta) - 1] . \end{aligned} \tag{3.46}$$

From Eqs. (3.45) and (3.46), we obtain the three-particle loop integral dispersion relation[12]

$$\mathrm{Re}\,[L_{\alpha\beta\gamma}(\omega)] = \frac{\mathcal{P}}{\pi} \int_{-\infty}^{\infty} d\omega' \eta_{\alpha\beta\gamma}(\omega')\ \frac{\mathrm{Im}\,[L_{\alpha\beta\gamma}(\omega')]}{(\omega' - \omega)} , \tag{3.47}$$

where

$$\eta_{\alpha\beta\gamma}(\omega_\gamma - \omega_\alpha - \omega_\beta) = \frac{N_{\alpha\beta\gamma}(\omega_\alpha, \omega_\beta, \omega_\gamma)}{D_{\alpha\beta\gamma}(\omega_\alpha, \omega_\beta, \omega_\gamma)} , \tag{3.48}$$

with

$$N_{\alpha\beta\gamma}(\omega_\alpha, \omega_\beta, \omega_\gamma) = \eta_\alpha(\omega_\alpha)\eta_\beta(\omega_\beta)\eta_\gamma(\omega_\gamma) - \eta_\alpha(\omega_\alpha) - \eta_\beta(\omega_\beta) + \eta_\gamma(\omega_\gamma) \tag{3.49}$$

and

$$D_{\alpha\beta\gamma}(\omega_\alpha, \omega_\beta, \omega_\gamma) = 1 + \eta_\alpha(\omega_\alpha)\eta_\beta(\omega_\beta) - \eta_\beta(\omega_\beta)\eta_\gamma(\omega_\gamma) - \eta_\alpha(\omega_\alpha)\eta_\gamma(\omega_\gamma) . \tag{3.50}$$

Then, for a finite-temperature causal function it can be shown from Eqs. (3.2) and (3.48)–(3.50) that

$$\eta_{\alpha\beta\gamma}(\omega) = \begin{cases} \tanh\{\omega - (\mu_\gamma - \mu_\alpha - \mu_\beta)/2k_\mathrm{B}T\} \\ \text{for three bosons or two fermions and one boson,} \\ \coth\{\omega - (\mu_\gamma - \mu_\alpha - \mu_\beta)/2k_\mathrm{B}T\} \\ \text{for three fermions or one fermion and two bosons.} \end{cases} \tag{3.51}$$

By comparing Eqs. (3.2), (3.40) and (3.51) we see a very satisfying physical result. The statistics for the loop depend upon the "statistical combination" of the particles making up the loop. For example, two fermions combine to form a boson, while the composite of three fermions is a fermion. Then, in the dispersion relations Eqs. (3.38) and (3.47) the appropriate η function is a tanh (with a suitable argument) for boson-like loops and a coth for fermion-like loops. Clearly, these results can be easily generalized to more complicated types of loop integrals.

4. The R and T Matrix Formalism in Momentum Space

We consider scattering solutions of the time-independent Schrödinger equation

$$(T+V)\Psi_E = E\Psi_E, \tag{4.1}$$

and T and V are the kinetic and potential energy operators, respectively. The solutions of Eq. (4.1) can be expressed in the Lippman–Schwinger form[51]

$$\Psi_E = \Phi_E + G_E V \Psi_E, \tag{4.2}$$

where Φ_E is a solution of the equation

$$(T-E)\Phi_E = 0, \tag{4.3}$$

and G_E is a Green's function involving the inverse of the operator $(T - E)$. In general, G_E will involve a PV operator.

To illustrate the PV formalism in these equations, we now specialize to momentum space. Also, we assume that V is essentially a *one-body potential,* which can arise in several types of problems. For example, one may have a two-body problem that clearly separates into center-of-mass and relative coordinates, so that the potential is a function only of the relative coordinate. Another possibility arises when many-body effects can be absorbed into a self-consistent single-particle potential. Moreover, we assume that the angular contributions can be removed from the formalism, with the wave function and operators decomposed into partial waves.

With these specializations, Eq. (4.2) becomes[60]

$$\psi_\ell^{(k_0)} = \phi_\ell^{(k_0)} + G_R^{(k_0)} V_\ell \psi_\ell^{(k_0)}, \tag{4.4}$$

where ℓ labels the angular momentum value, k_0 labels the energy

$$E = \frac{\hbar^2 k_0^2}{2m},$$

and $\phi_\ell^{(k_0)}$ is the ℓ-projected plane wave

$$\langle k \mid \phi_\ell^{(k_0)}\rangle = \phi_\ell^{(k_0)}(k) = N_\ell(k_0)\frac{\delta(k_0-k)}{k^2}, \tag{4.5}$$

with $N_\ell(k_0)$ a normalization factor. Note that the function on the right-hand side of Eq. (4.5) is essentially the nonangular part of the Fourier transform of a plane wave, which is a delta function,[5] namely

$$\delta(\mathbf{k}-\mathbf{k}_0) = \frac{\delta(k-k_0)}{k^2} \sum_{\ell m} Y^*_{\ell m}(\hat{k})\, Y_{\ell m}(\hat{k}_0), \tag{4.6}$$

where $Y_{\ell m}(\hat{k}) = Y_{\ell m}(\theta_k, \phi_k)$ is a spherical harmonic. Also, in Eq. (4.4) $V_\ell = V_\ell(k,k')$ is nonlocal in momentum space and $G_R^{(k_0)}$ is the Green's function.

$$G_R^{(k_0)}(k,k') = \frac{\mathcal{P}}{\frac{\hbar^2}{2m}(k_0^2-k^2)}\delta(k-k'). \tag{4.7}$$

It is easily verified that[51,60]

$$V_\ell \psi_\ell^{(k_0)} = R_\ell\, \phi_\ell^{(k_0)}, \tag{4.8}$$

where the R-matrix is given by

$$R_\ell = V_\ell + V_\ell\, G_R^{(k_0)}\, R_\ell, \tag{4.9}$$

or explicitly in matrix form

$$R_\ell(k,k_0) = V_\ell(k,k_0) - \frac{2m}{\hbar^2}\int_0^\infty dk' \frac{\mathcal{P}}{(k'^2-k_0^2)} k'^2\, V_\ell(k,k')\, R_\ell(k',k_0)\,. \tag{4.10}$$

In Appendix B we show how to solve Eq. (4.10) numerically.[29]

We can also define another Green's function[51,60]:

$$\begin{aligned} G_T^{(k_0)}(k,k') &= \left[\frac{\hbar^2}{2m}(k_0^2-k^2+i\varepsilon)\right]^{-1} \delta(k-k') \\ &= G_R^{(k_0)} - \frac{2m}{\hbar^2} i\pi\delta(k_0^2-k^2)\delta(k-k')\,, \end{aligned} \tag{4.11}$$

the last line of which follows from Eq. (2.5). We then have[60]

$$\chi_\ell^{(k_0)} = \phi_\ell^{(k_0)} + G_T^{(k_0)} V_\ell \chi_\ell^{(k_0)}, \tag{4.12}$$

$$V_\ell \chi_\ell^{(k_0)} = T_\ell \phi_\ell^{(k_0)} \tag{4.13}$$

and

$$T_\ell = V_\ell + V_\ell\, G_T^{(k_0)}\, T_\ell, \tag{4.14}$$

in analogy to Eqs. (4.4), (4.8) and (4.9).

From Eqs. (4.11) and (4.14), we find that the T matrix, T_ℓ, is given by

$$T_\ell(k,k_0) = V_\ell(k,k_0) - \frac{2m}{\hbar^2}\int_0^\infty dk' \left[\frac{\mathcal{P}}{(k'^2 - k_0^2)} k'^2 V_\ell(k,k')\, T_\ell(k',k_0) \right.$$
$$\left. - \, i\pi \frac{m}{\hbar^2} k_0 V_\ell(k,k_0) T_\ell(k_0,k_0) \right], \tag{4.15}$$

and, as before, we remove the PV, obtaining

$$T_\ell(k,k_0) = V_\ell(k,k_0) - \frac{2m}{\hbar^2}\int_0^\infty \frac{dk'}{(k'^2 - k_0^2)}$$
$$\times \Bigg\{ [\, k'^2\; V_\ell(k,k')\; T_\ell(k',k_0) - k_0^2\; V_\ell(k,k_0)\; T_\ell(k_0,k_0)]$$
$$- \, i\pi \frac{m}{\hbar^2} k_0 V_\ell(k,k_0)\; T_\ell(k_0,k_0) \Bigg\}. \tag{4.16}$$

In Appendix B, we also show how to determine the T-matrix in momentum space. For additional results involving the R and T matrices, see Refs. 28, 45 and 51.

5. Applications to Nuclear Physics

We now discuss some results from intermediate-energy nuclear physics, in which the loop integral in Fig. 1 is evaluated for nucleon-delta-pion interactions (see Refs. 12, 13, 16, 52 and 60). The aim is to solve iteratively Dyson's coupled equations for this system. There are two-loop integrals that are of great interest in the theory: (a) the nucleon-delta integral, which becomes a self-energy insertion into the pion Green's function or propagator, and (b) the nucleon-pion integral, which becomes a self-energy insertion into the delta particle Green's function.

In our model, we will assume that we are dealing with *infinite nuclear matter at zero temperature* with all propagators assumed to be causal. Also we will assume that the nucleon propagator, G_N, is taken from a *mean-field model*, with

$$G_N(\mathbf{p},\omega) = \frac{\Theta(e_N(p) - \mu_N)}{(\omega - e_N(p) + i\varepsilon)} + \frac{\Theta(\mu_N - e_N(p))}{(\omega - e_N(p) - i\varepsilon)}, \tag{5.1}$$

where $\mathbf{p}$ is the spatial momentum, with $p = |\mathbf{p}|$, and ω is the frequency (or energy); μ_N is the nucleon chemical potential. In Eq. (5.1), on the left-hand side we indicate a general dependence on $\mathbf{p}$, while the right-hand side in actuality involves p. This behavior will be true of all nuclear matter functions discussed in this section.[16] In this theory, we will also assume that the pion and delta propagators can change with iteration, but the nucleon propagator will always be specified by Eq. (5.1).

The mean-field energy in Eq. (5.1) is given by

$$e_N(p) = \frac{\hbar^2}{2m_N^*(\rho)} + V_N^{(0)}(\rho) + m_N c^2, \tag{5.2}$$

where m_N is the nucleon mass, and the effective nucleon mass, m_N^*, and mean-field potential, $V_N^{(0)}$, both depend on the nucleon matter density

$$\rho(p_\mathbf{F}) = \frac{2}{3\pi^2}\, p_\mathbf{F}^3, \tag{5.3}$$

with $p_\mathbf{F}$ the Fermi momentum. In Eq. (5.1), $\Theta(x)$ is the usual step function, while ε is infinitesimal, so that from Eq. (2.5) we obtain

$$(\omega - e_N(p) \pm i\varepsilon)^{-1} \underset{\varepsilon\to 0^+}{\longrightarrow} \frac{\mathcal{P}}{\omega - e_N(p)} \mp \delta(\omega - e_N(p))\,. \tag{5.4}$$

Reference 16 presents a method for calculating m_N^* and $V_N^{(0)}$, using a Skyrme-force model.

On the first iteration, we assume that the imaginary part of the delta particle propagator is given by[12,16]

$$\mathrm{Im}\,[G_\Delta(\mathbf{p},\omega)] = -\frac{1}{2}\frac{\Gamma_\Delta(\omega)\Theta(\omega-\mu_\delta)}{\left[(\omega - e_\Delta(p))^2 + \frac{1}{4}\Gamma_\Delta^2(\omega)\right]}, \tag{5.5}$$

where μ_Δ is the delta chemical potential and e_Δ is the delta mean-field energy

$$e_\Delta(p) = \frac{\hbar^2}{2m_\Delta^*(\rho)} + V_\Delta^{(0)}(\rho) + m_\Delta c^2, \tag{5.6}$$

with

$$\frac{m_\Delta^*(p)}{m_\Delta} = \frac{m_N^*(p)}{m_N} \tag{5.7}$$

and

$$V_\Delta^{(0)}(\rho) = V_N^{(0)}(\rho)\,. \tag{5.8}$$

The restriction in Eq. (5.5) to $\omega \geq \mu_\Delta$ is to prevent the propagation of holes. Reference 16 gives a prescription for calculating the delta width, $\Gamma_\Delta(\omega)$. Then, we calculate the real part of the delta propagation using Eqs. (3.1)–(3.3), giving

$$\mathrm{Re}\,[G_\Delta(\mathbf{p},\omega)] = \frac{\mathcal{P}}{\pi}\int_{-\infty}^{\infty} d\omega' \frac{\mathrm{Im}\,[G_\Delta(\mathbf{p},\omega')]\ \mathrm{sign}(\omega'-\mu_\Delta)}{(\omega'-\omega)}, \tag{5.9}$$

which can also be evaluated in closed form.[16] Equation (5.9) rigorously guarantees that causality is satisfied for the delta particle.

We can evaluate Eq. (3.36) in the limit of zero temperature,[12,16] to obtain

$$\begin{aligned}\mathrm{Im}[\mathcal{L}_{NA}(\mathbf{p},\omega)] = -2\int_{-\infty}^{\infty} d\omega' \int d^3\mathbf{q}\\ &\times [\Theta(\omega+\omega'-\mu_N)\Theta(\mu_\Delta-\omega') + \Theta(\mu_N-\omega-\omega')\Theta(\omega'-\mu_\Delta)]\\ &\times [F(|2\mathbf{q}+\mathbf{p}|, 2\omega'+\omega)]^2 \mathrm{Im}[G_N(\mathbf{p}+\mathbf{q},\omega+\omega')]\mathrm{Im}[G_\Delta(\mathbf{q},\omega')],\end{aligned} \tag{5.10}$$

where we have also made two generalizations: (a) including a three-dimensional spatial momentum integral that is "covariant" with the frequency integral and (b) inserting the form factor

$$F(\mathbf{p},\omega) = \frac{A}{(\omega^2 + |\mathbf{p}|^2)^2 + B}; A, B \text{ consts},$$

in order to assure convergence of the analogous nucleon–pion loop integral (to be discussed). We emphasize that in Eq. (5.10) the form factor is not really crucial for convergence. However, it is necessary in the nucleon–pion integral, for consistency, it can also be used in the nucleon–delta integral.

We recall that the nucleon–delta loop integral is to be inserted as a self-energy correction into the pion propagator. The actual insertion involves several additional manipulations.[16,52] First, we must define

$$\mathrm{Im}\left[U^{(0)}_{N\Delta}(\mathbf{p},\omega)\right] = \mathrm{Im}\left[\mathcal{L}_{N\Delta}(\mathbf{p},\omega)\right] + \mathrm{Im}\left[\mathcal{L}_{N\Delta}(-\mathbf{p},\omega)\right] . \tag{5.11}$$

Then, from Eqs. (3.38)–(3.41) we find, in the zero temperature limit, that

$$\mathrm{Im}\left[U^{(0)}_{N\Delta}(\mathbf{p},\omega)\right] = \frac{\mathcal{P}}{\pi}\int_{-\infty}^{\infty} d\omega' \frac{\mathrm{Im}\left[U^{(0)}_{N\Delta}(\mathbf{p},\omega')\right]\ \mathrm{sign}(\omega')}{(\omega' - \omega)}, \tag{5.12}$$

in which we have also assumed that

$$\mu_\Delta = \mu_N,$$

which appears to be satisfied for densities up to about twice normal nuclear matter density.[16] As before, Eq. (5.12) guarantees that causality is rigorously satisfied for the pion self-energy correction. Next, the *full vertex* correction is given by[16,52]

$$U_{N\Delta}(\mathbf{p},\omega) = \left[1 + sU^{(0)}_{N\Delta}(\mathbf{p},\omega)\right]^{-1} U^{(0)}_{N\Delta}(\mathbf{p},\omega), \tag{5.13}$$

where

$$s = \frac{8\pi^2}{9(\hbar c)m^*_N p_\mathrm{F}} g'_\Delta$$

and $g'_\Delta = 0.45$ is the Migdal parameter.[16] In practice, it has been found that $U_{N\Delta}$ and $U^{(0)}_{N\Delta}$ differ negligibly.[16] The largest difference is ≈ 10 % for $p \leq 1.0\ \mathrm{fm}^{-1}$, with the discrepancy decreasing with increasing p.

Finally, the explicit expression the pion propagator, including the self-energy insertion from the nucleon-delta loop integral, is

$$D(\mathbf{p},\omega) = \left[1 - D_0(\mathbf{p},\omega)\Sigma_\pi(\mathbf{p},\omega)\right]^{-1} D_0(\mathbf{p},\omega), \tag{5.14}$$

where

$$D_0(\mathbf{p},\omega) = (\omega^2 - p^2c^2 - m_\pi^2c^4 + i\varepsilon)^{-1} \tag{5.15}$$

is the usual free-particle casual pion propagation (with ε infinitesimal), and

$$\Sigma_\pi(\mathbf{p},\omega) = -\frac{16}{9}(\hbar c)^2 \left(\frac{f^*}{m_\pi}\right)^2 U_{N\Delta}(\mathbf{p},\omega); \quad (f^*)^2 = 1.28\pi, \tag{5.16}$$

is a "polarization" operation.[16]

After a series of additional manipulations, a pion–nucleon loop integral, $\Sigma_\Delta^{(0)}(\mathbf{p},\omega)$, can be defined in analogy with Eq. (5.10). However, in this integral the pion propagator is multiplied by an additional function involving $U_{N\Delta}(\mathbf{p},\omega)$. Also, as mentioned before, for this loop integral the form factor is crucial for obtaining convergence. Then, after the imaginary part of $\Sigma_\Delta(\mathbf{p},\omega)$ is computed, we obtain its real part from

$$\mathrm{Re}\left[\Sigma_\Delta^{(0)}(\mathbf{p},\omega)\right] = \frac{\mathcal{P}}{\pi}\int_{-\infty}^{\infty} d\omega' \frac{\mathrm{Im}\left[\Sigma_\Delta(\mathbf{p},\omega')\right]\ \mathrm{sign}(\omega'-\mu_N)}{(\omega'-\omega)} \tag{5.17}$$

and $\Sigma_\Delta^{(0)}(\mathbf{p},\omega)$ is inserted into an iterated delta propagator[16]:

$$[G_\Delta(\mathbf{p},\omega)]^{-1} = \omega - e_\Delta(p) - \Sigma_\Delta^{(0)}(\mathbf{p},\omega)\,. \tag{5.18}$$

Thus, $\Sigma_\Delta^{(0)}(\mathbf{p},\omega)$ is the exact self-energy correction to the delta propagator. Then, in principle the entire process outlined above can be repeated, until we achieve some type of self-consistency. Here we just deal with the first iteration. The imaginary and real parts of $U_{N\Delta}(\mathbf{p},\omega)$ versus ω are plotted in Figs. 3 and 4, respectively, for five different p values.[16] The curves $\mathrm{Re}(U_{N\Delta})$'s have the expected kind of behavior for functions computed from the dispersion relation, Eq. (5.12). That is, for functions behaving as in Fig. 3, their dispersion relation "partners" have the types of shapes displayed in Fig. 4.

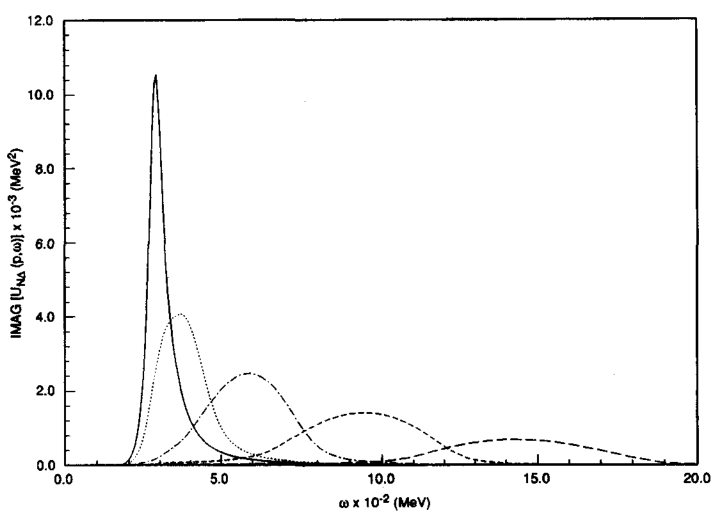

Fig. 3. The Im $[U_{N\Delta}(p,\omega)]$ vs ω for $p = 0, 2, 4, 6$ and 8 fm^{-1} (the full, dotted, dot-dashed, short-dashed, and long-dashed curves, respectively).

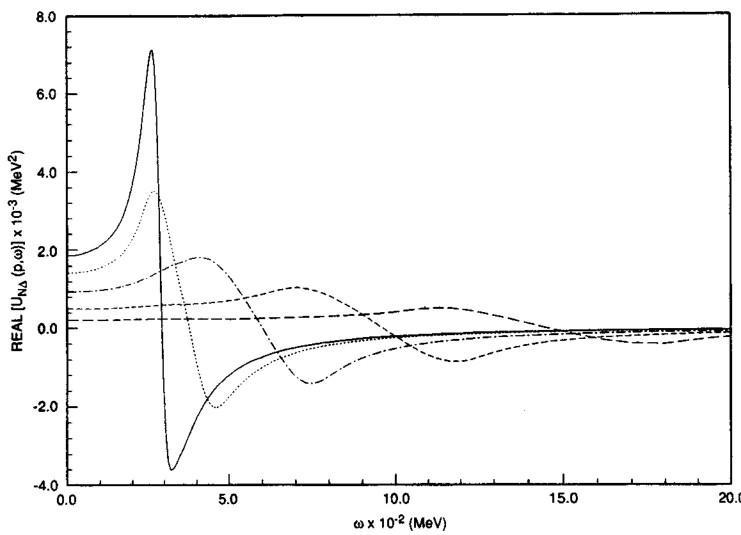

Fig. 4. The Re $[U_{N\Delta}(p,\omega)]$ vs ω, for various p values. The conventions for the curves are the same as in Fig. 3.

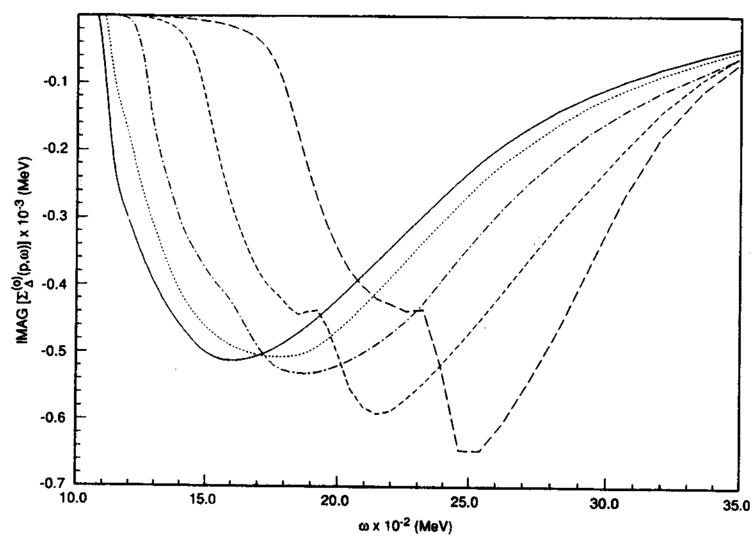

Fig. 5. The Im $\left[\Sigma_\Delta^{(0)}(p,\omega)\right]$ vs ω, for $p = 1, 3, 5, 7$ and $9\ \mathrm{fm}^{-1}$ (the full, dotted, dot-dashed, short-dashed, and long-dashed curves, respectively).

The imaginary and real parts of $\Sigma_\Delta^{(0)}(\mathbf{p},\omega)$ are plotted in Figs. 5 and 6 (see Ref. 16). Again, the dispersion relation partners displayed in Figs. 5 and 6 have the expected shapes. However, we note that the behavior with respect to p shown in Figs. 5 and 6 is very different from that shown in Figs. 3 and 4.

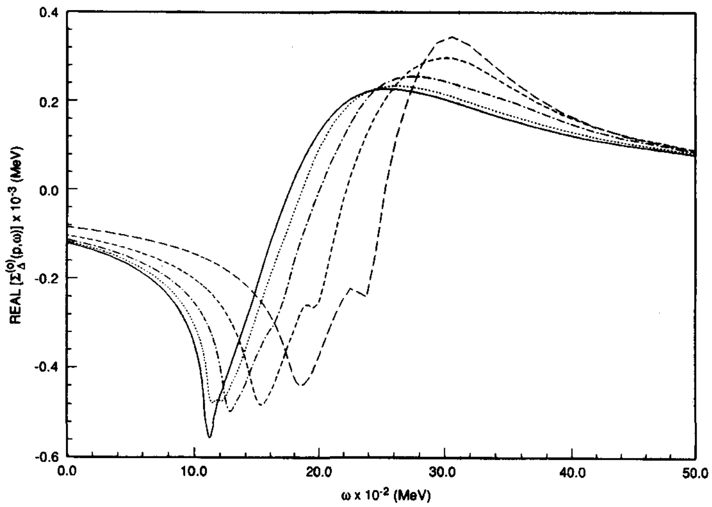

Fig. 6. The Re $\left[\Sigma_{\Delta}^{(0)}(p,\omega)\right]$ vs ω, for several p values. The conventions for the curves are the same as in Fig. 5.

In any case, here we are not trying to resolve the complicated questions in the theory of pion-nucleon-delta-interactions. Our main purpose is to show that the formalism of two-particle loop integrals, discussed in Sec. 3.3, has applications to real nuclear physics problems. In turn, this formalism can be derived, as shown previously, using the PB theorem, which shows once again that the theorem is applicable to many types of problems in physics.

6. Applications to Transport Theory

Transport equations describe the rate of change of macroscopic physical quantities (e.g. number of particles, density, energy, electric charge) due to convection, leakage, absorption, etc. The fundamental transport equation was postulated by Boltzmann in 1872 to describe the temporal evolution of the one-particle distribution function of a rarefied gas with binary collisions.[3] Thenceforth the nonlinear integro-differential Boltzmann equation has become the paradigm of transport equations and has been adapted, simplified, generalized, or extended to cover various situations. For instance, linear or linearized approximations are used for neutron transport and gases close to equilibrium. Grazing collisions that occur in electron scattering lead to small angle expansions and the ensuing Fokker–Planck type equations. Applications to charged particles introduce nonlinearities in the convection term itself (as opposed to the collision term) and are treated in the Vlasov equation formalism. Inclusion of several species of particles form systems of coupled Boltzmann equations, finite size effects are taken into account within the Enskog approximation, and higher order collisions that take place in denser gases can also be accommodated. The interested reader can find the basic principles of transport

equations and their developments in one of the excellent monographs in this field (see Refs. 8, 9 and 19, and references therein).

It is beyond the scope of this section to review all the situations described by transport theory whereby the PB formula or its generalizations can be applied. Instead, we shall restrict ourselves to illustrate these applications to a couple of simple examples that also bear historical significance. Since the collisionless Vlasov equation and the monoenergetic neutron transport were the first two transport problems where the PB formula has been recognized, (sometimes) rederived, and applied, we shall focus on these cases.

6.1. *Collisionless electron plasma*

In the framework of transport theory, the electron plasma is a charged gas described by the one-particle distribution function $f_0(v) + f(\mathbf{r}, \mathbf{v}, t)$. Here $f_0(v)$ is the equilibrium distribution function, which is assumed to depend only on the magnitude, v, of the velocity $\mathbf{v}$, while $f(\mathbf{r}, \mathbf{v}, t)$ describes the perturbation, depending on position $\mathbf{r}$, velocity $\mathbf{v}$, and time t. The ansatz $f_0 = f_0(v)$ is equivalent to saying that equilibrium state is homogeneous and isotropic. Assuming that the plasma is very rarefied (i.e. it is in the collisionless or Vlasov regime) and linearizing around f_0, the transport equation for the electron gas can be written as[6,33]:

$$\frac{\partial f}{\partial t} + \mathbf{v}\frac{\partial f}{\partial \mathbf{r}} + \frac{e}{m}\mathbf{E}\frac{\partial f_0}{\partial \mathbf{v}} = 0\,, \tag{6.1}$$

$$\mathbf{E}(\mathbf{r}, t) = e\int \frac{\mathbf{r} - \mathbf{r}'}{\mid \mathbf{r} - \mathbf{r}'^3 \mid} d\mathbf{r}' \int f(\mathbf{r}', \mathbf{v}', t)\ d\mathbf{v}', \tag{6.2}$$

where e denotes the electron charge and m its mass. Looking for solutions of the form:

$$f(\mathbf{r}, \mathbf{v}, t) \sim e^{i\mathbf{r}\cdot\mathbf{k}} e^{-i\omega t}\ \phi_{k,\omega}(\mathbf{v}), \tag{6.3}$$

we obtain

$$(\omega - \mathbf{k}\cdot\mathbf{v})\phi_{k,\omega}(\mathbf{v}) = -\frac{4\pi e^2}{m}\frac{\mathbf{k}\cdot\mathbf{v}}{k^2 v}\ \frac{\partial f_0}{\partial v}\int \phi_{k,\omega}(\mathbf{v}')d\mathbf{v}'. \tag{6.4}$$

Equation (6.4) can be further simplified. We take $\mathbf{k}$ as the z-axis, denote $\frac{\mathbf{k}\cdot\mathbf{v}}{k} = v_z \equiv u$, integrate over v_x, v_y, and use the identity

$$\int_{-\infty}^{\infty} dv_x \int_{-\infty}^{\infty} dv_y \frac{1}{v}\frac{\partial f_0}{\partial v} = -2\pi f_0(u) \tag{6.5}$$

to find

$$(\omega - ku)\overline{\phi}_{k,\omega}(u) = \eta_k(u)\int_{-\infty}^{\infty} \overline{\phi}_{k,\omega}(u')du', \tag{6.6}$$

where

$$\overline{\phi}_{k,\omega}(u) = \int_{-\infty}^{\infty} dv_x \int_{-\infty}^{\infty} dv_y\ \phi_{k,\omega}(\mathbf{v}) \tag{6.7}$$

and

$$\eta_k(u) = \frac{8\pi^2 e^2}{m}\frac{u}{k} f_0(u)\,. \tag{6.8}$$

The integral $\int_{-\infty}^{\infty} \overline{\phi}_{k\omega}(u')du'$ cannot be zero; indeed, assuming that this quantity vanishes, we find that $\overline{\phi}(u) = \delta(\omega - ku)$ and thus

$$\int_{-\infty}^{\infty} \overline{\phi}_{k,\omega}(u)du \neq 0,$$

yielding a contradiction. Thus we may normalize the integral to one. With this choice, there are two classes of solutions[6,30] for Eq. (6.6):
Class 1.

$$\overline{\phi}_{k,\omega}(u) = \frac{\eta_k(u)}{\omega - ku}, \tag{6.9}$$

for all the *discrete* ω that satisfy the equation:

$$\Lambda_k(\omega) \equiv 1 - \int_{-\infty}^{\infty} \frac{\eta_k(u)}{\omega - ku}du = 0\,. \tag{6.10}$$

The function $\Lambda_k(\omega)$ is usually called the plasma dispersion function.
Class 2.

$$\overline{\phi}_{k,\omega}(u) = \left[\mathcal{P}\frac{\eta_k(u)}{\omega - ku} + \lambda(k,\omega)\delta(\omega - ku)\right]. \tag{6.11}$$

The arbitrariness in choosing $\lambda(k,\omega)$ can be utilized to get a complete set of functions and to satisfy the normalization constraints. The latter implies that $\overline{\phi}_{k,\omega}(u)$ does not contain other singular terms — for instance derivatives of the δ-function. The normalization condition $\int_{-\infty}^{\infty} \overline{\phi}_{k,\omega}(u)du = 1$ yields $\lambda(k,\omega) = 1 - \mathcal{P}\int_{-\infty}^{\infty} \frac{\eta_k(u)}{\omega - ku}du$.

The generalized eigenfunctions (6.11) are complete and satisfy orthogonality relations in the form[7,30]:

$$\int_{-\infty}^{\infty} \overline{\phi}_{k,\omega}(u)\overline{\phi}_{k,\omega'}(u)\eta_k^{-1}(u)du = N(k,\omega)\delta(\omega - \omega')\,. \tag{6.12}$$

To compute the normalization factor $N(k,\omega)$, one applies the PB formula which yields[7]:

$$N(k,\omega) = \frac{\lambda^2(k,\omega) + \pi^2\eta_k^2(\omega/k)}{\eta_k(\omega/k)}. \tag{6.13}$$

We shall give more details of the application of the PB formula in Sec. 6.2.

6.2. *Monoenergetic neutron transport*

The neutron transport equation describes the advection, absorption, and production of neutrons in a host medium. The interest in this application grew dramatically

during and after WWII in relation with civilian and military applications (nuclear reactors and atomic bombs, respectively).

The neutron gas is neutral and is assumed to collide only with the host medium. Thus, the corresponding transport equation is linear. Moreover, we shall assume, for simplicity, that the transport is stationary, the scattering is isotropic, the neutrons are monoenergetic, and the geometry is one-dimensional. Under these assumptions, the Boltzmann equation can be written[6,34]

$$\mu\frac{\partial f}{\partial x} + f = \frac{c}{2}\int_{-1}^{1} f(x,\mu')d\mu', \tag{6.14}$$

where $f(x,\mu)$ is the stationary one-particle distribution function depending on position x and cosine μ of the angle made by the velocity with the x-axis. In Eq. (6.14) the neutrons' speed and the absorption cross-section are normalized to one. The constant c describes the multiplication properties of the medium ($c < 1-$ subcritical; $c = 1-$ critical; $c > 1-$ supercritical). We restrict ourselves to the case $c < 1$ and look for solutions in the form:

$$f(x,\mu) = e^{-x/\nu}\phi_\nu(\mu)\,, \tag{6.15}$$

which leads to

$$(\nu-\mu)\phi_\nu(\mu) = \frac{c\nu}{2}\int_{-1}^{1}\phi_\nu(\mu')d\mu'. \tag{6.16}$$

Since $\int_{-1}^{1}\phi_\nu d\mu$ cannot be zero (see the argument after Eq. (6.8)), we normalize it to one and obtain again two classes of solutions:
Class 1.

$$\phi_{\nu_i}(\mu) = \frac{c\nu_i}{2}\frac{1}{\nu_i-\mu}, \tag{6.17}$$

where the two discrete roots $\nu_i \notin [-1,1]$ are the solutions of the dispersion equation

$$\Omega(\nu) \equiv 1 - \frac{c\nu}{2}\int_{-1}^{1}\frac{1}{\nu-\mu}d\mu = 0. \tag{6.18}$$

Class 2. For $\nu \in [-1,1]$ we get

$$\phi_\nu(\mu) = \frac{c\nu}{2}\mathcal{P}\frac{1}{\nu-\mu} + \lambda(\nu)\delta(\nu-\mu)\,. \tag{6.19}$$

These generalized eigenfunctions satisfy the orthogonality relations

$$\int_{-1}^{1}\mu\;\phi_\nu(\mu)\phi_{\nu'}(\mu)d\mu = N(\nu)\delta(\nu-\nu')\,. \tag{6.20}$$

To obtain the normalization factor, $N(\nu)$, for the continuum modes, we follow essentially the derivation in Ref. 8. The expansion of an arbitrary function $f(\mu)$ in the continuum modes reads

$$f(\mu) = \int_{-1}^{1} A(\nu')\phi_{\nu'}(\mu)d\nu'. \tag{6.21}$$

Multiplying by $\mu\phi_\nu(\mu)$ and integrating over μ, we get

$$\int_{-1}^{1} \mu\phi_\nu(\mu) f(\mu) d\mu = \int_{-1}^{1} \mu\phi_\nu(\mu) d\mu \left(\int_{-1}^{1} A(\nu')\phi'_\nu(\mu) d\nu' \right). \tag{6.22}$$

The left-hand side of Eq. (6.22) is defined to be the product between the expansion coefficient $A(\nu)$, and the normalization factor $N(\nu)$. The double integral on the right-hand side is evaluated by using the PB formula. Carrying this out, Eq. (6.22) becomes

$$\begin{aligned} N(\nu)A(\nu) &= \int_{-1}^{1} \mu d\mu \left[\frac{c\nu}{2} \frac{\mathcal{P}}{\nu - \mu} + \lambda(\nu)\delta(\nu - \mu) \right] \\ &\quad \times \left(\int_{-1}^{1} A(\nu') \left[\frac{c\nu'}{2} \frac{\mathcal{P}}{\nu' - \mu} + \lambda(\nu')\delta(\nu' - \mu) \right] d\nu' \right) \\ &= \int_{-1}^{1} d\mu\mu \frac{c\nu}{2} \frac{\mathcal{P}}{\nu - \mu} \int_{-1}^{1} A(\nu') \frac{c\nu'}{2} \frac{\mathcal{P}}{\nu' - \mu} d\nu' \\ &\quad + \int_{-1}^{1} d\mu\mu\lambda(\nu)\delta(\nu - \mu) \int_{-1}^{1} A(\nu') \frac{c\nu'}{2} \frac{\mathcal{P}}{\nu' - \mu} d\nu' \\ &\quad + \int_{-1}^{1} d\mu \frac{c\nu}{2} \frac{\mathcal{P}}{\nu - \mu} \int_{-1}^{1} A(\nu')\lambda(\nu')\delta(\nu' - \mu) d\nu' \\ &\quad + \int_{-1}^{1} d\mu\mu\lambda(\nu)\delta(\nu - \mu) \int_{-1}^{1} A(\nu')\lambda(\nu')\delta(\nu' - \mu) d\nu'. \end{aligned} \tag{6.23}$$

The last three terms in Eq. (6.23) are computed without difficulty, yielding:

$$\begin{aligned} &\frac{c\nu}{2}\lambda(\nu) \int_{-1}^{1} \frac{\mathcal{P}}{\nu' - \nu} A(\nu')\nu' d\nu' \\ &\qquad - \frac{c\nu}{2} \int_{-1}^{1} \frac{\mathcal{P}}{\nu' - \nu} A(\nu')\lambda(\nu')\nu' d\nu' + \nu\lambda(\nu)\lambda^2(\nu). \end{aligned} \tag{6.24}$$

From the first term, by applying the PB formula (2.35) and identifying $f(\mu, \nu')$ with $\frac{c^2\nu\nu'}{4}\mu A(\nu')$, we get

$$\begin{aligned} &\int_{-1}^{1} d\mu \frac{\mathcal{P}}{\nu - \mu} \int_{-1}^{1} d\nu' \frac{\mathcal{P}}{\nu' - \mu} \frac{c^2\nu\nu'}{4} \mu A(\nu') \\ &\qquad = \pi^2 \frac{c^2\nu^3}{4} A(\nu) + \int_{-1}^{1} d\nu' \int_{-1}^{1} \frac{\mathcal{P}}{\nu - \mu} \frac{\mathcal{P}}{\nu' - \mu} \frac{c^2\nu\nu'}{4} \mu A(\nu') d\mu. \end{aligned} \tag{6.25}$$

In (6.25) we make use of the identity

$$\mu \frac{\mathcal{P}}{\nu - \mu} \frac{\mathcal{P}}{\nu' - \mu} = \left[\nu \frac{\mathcal{P}}{\nu - \mu} - \nu' \frac{\mathcal{P}}{\nu' - \mu} \right] \frac{\mathcal{P}}{\nu' - \nu} \tag{6.26}$$

to get

$$\frac{c^2}{4}\nu \int_{-1}^{1} \frac{\mathcal{P}}{\nu' - \nu}\nu' A(\nu')d\nu' \int_{-1}^{1} d\mu \left[\nu\frac{\mathcal{P}}{\nu - \mu} - \nu'\frac{\mathcal{P}}{\nu' - \mu}\right]$$
$$= \frac{c^2}{4}\nu \int_{-1}^{1} \frac{\mathcal{P}}{\nu' - \nu}\left[\frac{2}{c}(\lambda(\nu') - \lambda(\nu))\right]\nu' A(\nu')d\nu'. \tag{6.27}$$

When collecting the results, the terms in (6.27) cancel the first two terms in (6.24). Eventually, we obtain $N(\nu)A(\nu) = \nu A(\nu)\lambda^2(\nu) + \pi^2\frac{c^2\nu^3}{4}A(\nu)$, which yields

$$N(\nu) = \nu\left[\lambda^2(\nu) + \frac{\pi^2 c^2 \nu^2}{4}\right]. \tag{6.28}$$

A similar derivation was used to obtain (6.13). Other applications of the PB formula to transport theory can be found in Refs. 36 and 43. Related applications to the half-Hilbert and half-Hartley transforms have been recently discussed in Ref. 50.

7. PV Integrals in Condensed Matter Physics

Because the electron energy distribution in many solids is continuous in character, multidimensional PV integrals arise naturally in calculations relating to condensed matter physics. This is particularly the case for those of a perturbative nature, where vanishing energy denominators are the rule. Due to the need for high accuracy in distinguishing subtle features, the numerical treatment of these integrals has often strained the limits of computational technology. In spite of this, some results remained tainted with controversy until exact analytical evaluations were achieved. Even in discrete lattice problems what is interesting, in many cases, is the real part of a causal Green function, often best expressed as a PV integral over a polyhedral domain in reciprocal space. This section contains several examples of such principal value calculations important in solid state theory, and their analytical resolution. In each case, the interesting features are the means by which the singularity in the integrand is treated analytically and the intricate analytic structure revealed.

Forty years ago, Lindhard[38] evaluated the density response function for the non-interacting homogeneous electron gas, $\Pi_0(k,\omega)$ — one of the fundamental quantities in the theory of metals — represented by a Feynman diagram similar to the one in Fig. 1.

A formal expression for the lowest order corrections, due to Coulomb interactions among the electrons, corresponds to the sum of three diagrams like the one in Fig. 1, two with Coulomb self-energy parts in one of the two propagators, and the third having a vertex correction connecting the two propagators. This was worked out for the first time by Dubois[18] in 1959. In the static case ($\omega = 0$), in suitably scaled form, this is proportional to the six-dimensional PV integral

$$I(q) = \mathcal{P}\int_{\mathcal{R}} \frac{d^3\mathbf{k}}{(\mathbf{k}\cdot\mathbf{q})^2}\int_{\mathcal{R}'} \frac{d^3\mathbf{k}'}{(\mathbf{k}'\cdot\mathbf{q})^2}\left\{\left[\frac{\mathbf{q}\cdot(\mathbf{k}+\mathbf{k}')}{|\mathbf{k}+\mathbf{k}'|}\right]^2 - \left[\frac{\mathbf{q}\cdot(\mathbf{k}-\mathbf{k}')}{|\mathbf{k}-\mathbf{k}'|}\right]^2\right\}. \tag{7.1}$$

Here, $\mathcal{R}$ is the region $\{\mathbf{k}||\mathbf{k}-\frac{1}{2}\mathbf{q}|<1\}$. The numerical study of $I(q)$ began with Geldart and Taylor,[25] who used the Pauli principle to isolate the singularity and were able to calculate the result in the range $0<q<2$. Because of questions concerning gradient terms in density functional theory, the precise behavior at $q=0$ and $q=2$ is required. In 1990 Engel and Vosko[20] derived the analytic expression

$$I(q) = -\frac{1-q^4}{48q^3}\left(\ln\left|\frac{1+q}{1-q}\right|\right)^3 + \frac{1-q^2}{24q^2}\int_0^q dx\frac{1-x^2}{x^2}\left(\ln\left|\frac{1+x}{1-x}\right|\right)^3$$
$$-\frac{1}{8}\left(\frac{1}{q}+\frac{1-q^2}{2q^2}\ln\left|\frac{1+q}{1-q}\right|\right)\int_0^q dx\frac{1-x^2}{x^2}\left(\ln\left|\frac{1+x}{1-x}\right|\right)^2. \tag{7.2}$$

The method used to obtain (7.2) was to decompose $I(q)$, defined in (7.1), into four integrals, two with denominators $(\mathbf{k}\cdot\mathbf{q})^2(\mathbf{k}\pm\mathbf{k}')^2$, which can be evaluated easily in terms of spherical coordinates, and two with denominators $(\mathbf{k}\cdot\mathbf{q})(\mathbf{k}'\cdot\mathbf{q})(\mathbf{k}\pm\mathbf{k}')^2$, which cannot. The first of these, $A_-(q)$, is even in q and reduces easily to a fourfold PV integral in cylindrical coordinates. Engel and Vosko then showed that it satisfies the differential equation

$$DA_- = \frac{q}{1-q^2}\ln\left|\frac{1+q}{1-q}\right| \tag{7.3}$$

with boundary condition $\lim_{q\to\infty} q^4 A_-(q) = \text{const}$, where D is the differential operator

$$\frac{d}{dq}(1-q^2)\frac{d}{dq}q^3\frac{d}{dq}. \tag{7.4}$$

The unique solution to this problem is found directly. The attempt to carry this procedure out for the second integral, $A_+(q)$, failed due to the more complex q dependence of the integrand. To get around this, Engel and Vosko expanded $\bar{A}_+(q)$ to order q^{-8} for large q and noted that the resulting series is, to that order, consistent with the differential equation

$$DA_+(q) = \frac{1}{q(1-q^2)}\ln\left|\frac{1+q}{1-q}\right|, \tag{7.5}$$

for which the unique solution can again be found directly. Thus, while the derivation of (7.2) relies on the unproven assumption (7.5), there is little doubt that it is indeed exact, since it reproduces all previously known information about $I(q)$. Recently, (7.1) has been evaluated exactly[27] by the reduction of (7.1) to a single integral which can be evaluated in terms of PV integrals of elementary functions and polylogarithms.[40] The PV singularity in terms where it could not be eliminated was evaluated by means of the definition. Wherever possible, it was first reduced to a logarithmic (and therefore integrable) singularity through integration by parts producing integrals with one logarithm in the integrand, leading to the Euler dilogarithm, and integrals with two logarithms, leading to the trilogarithm. The result,

for $0 < k < 2$, is

$$\begin{aligned}
I(k) &= \frac{1}{16k^2}\left[4k - (4-k^2)\ln\left(\frac{2-k}{2+k}\right)\right]\left\{\frac{1}{2}\left[(2-k)\ln^2\left(\frac{2-k}{2}\right)\right.\right.\\
&- \left.(2+k)\ln^2\left(\frac{2+k}{2}\right)\right] + (2+k)\ln\left(\frac{2+k}{2}\right)\ln\left(\frac{2-k}{2}\right)\\
&- 4\ln(2)\ln\left(\frac{2-k}{2}\right) - \frac{1}{k}(2-k)\ln^2\left(\frac{2-k}{2+k}\right)\\
&+ 4\left[\mathrm{Li}_2\left(\frac{2k}{2+k}\right) + \mathrm{Li}_2\left(\frac{2+k}{4}\right)\right] + 2\ln^2(2) - \pi^2/3\Big\} - \frac{1}{24k^2}(4-k^2)\\
&\times\left\{\frac{1}{4k}(4+k^2)\ln^3\left(\frac{2-k}{2+k}\right) - 6(1-\ln(2))\ln^2\left(\frac{2+k}{k}\right)\right.\\
&- \frac{1}{k}\left[(2+k)\ln^3\left(\frac{2+k}{k}\right) - (2-k)\ln^3\left(\frac{2-k}{k}\right)\right]\\
&-\frac{3}{k}\left[(2-k)\ln^2\left(\frac{2-k}{k}\right) - (2+k)\ln^2\left(\frac{2+k}{k}\right)\right] - 6\ln\left(\frac{2+k}{2k}\right)\ln^2\left(\frac{2-k}{2+k}\right)\\
&- \frac{3}{k}(2-k)\left[\ln\left(\frac{2-k}{k}\right)\ln\left(\frac{2+k}{k}\right) - \ln\left(\frac{4-k^2}{k^2}\right)\right]\ln\left(\frac{2-k}{2+k}\right)\\
&- \frac{1}{2}\left[(2+k)\ln^3\left(\frac{2+k}{2}\right) + (2-k)\ln^3\left(\frac{2-k}{2}\right)\right] - 6\ln^2(2)\ln\left(\frac{2+k}{k}\right)\\
&+ 2\ln^3\left(\frac{2+k}{2k}\right) + 6\ln(2)(2-\ln(2))\ln\left(\frac{4-k^2}{4}\right)\\
&+ \frac{3}{2}\ln\left(\frac{2-k}{2}\right)\ln\left(\frac{2+k}{2}\right)[(2+k)\ln(2+k) + (2-k)\ln(2-k) - 4]\\
&- 6\ln\left(\frac{2+k}{4}\right)\ln\left(\frac{2-k}{4}\right)\ln\left(\frac{4-k^2}{16}\right) + 12\left[\ln\left(\frac{2-k}{2+k}\right)\mathrm{Li}_2\left(\frac{2-k}{2+k}\right)\right.\\
&- \left.\ln\left(\frac{2+k}{4}\right)\mathrm{Li}_2\left(\frac{2+k}{4}\right)\right] - (1-\ln(2))\left[\mathrm{Li}_2\left(\frac{2+k}{4}\right) + \mathrm{Li}_2\left(\frac{2-k}{4}\right)\right]\\
&+ 12\left[\mathrm{Li}_3\left(\frac{2+k}{4}\right) + \mathrm{Li}_3\left(\frac{2-k}{4}\right) - \mathrm{Li}_3\left(\frac{2-k}{2+k}\right)\right]\\
&+ \left.2\pi^2(1-\ln(2)) - 12\ln^2(2) + 10\ln^3(2) - 9\zeta(3)\right\}. \qquad (7.6)
\end{aligned}$$

By examining this formidable expression, one can appreciate the intricate analytic complexity lurking behind the PV symbol, which is frequently missed in numerical studies. By comparing (7.6) with (7.2), expressions for Engel and Vosko's integrals were deduced and proven by symbolic differentiation, thereby proving the validity of the assumption on which (7.2) is based.

Let us now turn to the second class of problems which result in multidimensional PV integrals. Consider a regular lattice for which the nearest neighbors to a given lattice point, which we assume to be the origin, are $\boldsymbol{\delta}_1, \ldots, \boldsymbol{\delta}_c$. The corresponding lattice Green function is then the solution to the difference equation

$$zG(z;\mathbf{r}) - \sum_{j=1}^{c} J_j G(z;\mathbf{r}+\boldsymbol{\delta}_j) = \delta_{\mathbf{r},\mathbf{0}}\,, \tag{7.7}$$

where z is a complex parameter and J_j is a fixed "bond strength". This function can be expressed formally as

$$G(z;\mathbf{r}) = \frac{1}{\Omega}\int d\mathbf{k}\frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{z-\omega(\mathbf{k})}\,,$$
$$\omega(\mathbf{k}) = \sum_{j=1}^{c} J_j e^{i\mathbf{k}.\boldsymbol{\delta}_j}\,, \tag{7.8}$$

where the integral is over the unit cell of the reciprocal lattice, having volume Ω. These functions play a central role in crystal physics where one generally writes[42] $z = t - i\varepsilon$ with t real and ε infinitesimal. The imaginary part

$$\rho(t) = \frac{1}{\pi}\,\mathrm{Im}\;G(t-i\varepsilon;\mathbf{0}) \tag{7.9}$$

plays the role of a density of states, while the real part

$$g(t;\mathbf{r}) = \frac{\mathcal{P}}{\Omega}\int d\mathbf{k}\frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{t-\omega(\mathbf{k})} \tag{7.10}$$

acts as a generating function for transport paths for elementary excitations on the lattice. In particular, $g(\sum_{j=1}^{c} J_j, \mathbf{0})$ is directly related to the probability that a lattice excitation eventually returns to its starting point. The high precision evaluation of these PV integrals for lattices in three and higher dimensions is extremely difficult and is the subject of hundreds of studies since special cases for the three cubic lattices were first worked out exactly in a classic paper by G. N. Watson[58] in 1939. Unfortunately, no comprehensive review of these studies is available, but the earlier work is surveyed and documented in Ref. 32. Here we shall look at exact expressions for the "simple cubic" lattices ($J_j = 1$) in various dimensions.

In one and two dimensions the PV can be found by analytic continuation. We have, in the one-dimensional case,

$$g(t,n) = \frac{1}{\pi}\,\mathrm{Re}\int_0^{\pi}\frac{\cos(nx)}{t-i\varepsilon-\cos(x)}. \tag{7.11}$$

Now, for $t > 1$ the integral is $\pi[t-\sqrt{t^2-1}]^n/\sqrt{t^2-1}$, so by analytic continuation to $0 < t < 1$, we find

$$g(t;n) = -\frac{\mathrm{Im}\;\left[t+i\sqrt{1-t^2}\right]^n}{\sqrt{1-t^2}} = -\frac{U_n(t)}{\sqrt{1-t^2}}, \tag{7.12}$$

where $U_n(t)$ is a Tchebyshev polynomial of the second kind. Note that the corresponding Watson integral $(n = 0, t = 1)$ does not exist.

In two dimensions, the Green function is

$$G(t,(m,n)) = \frac{1}{\pi^2}\int_0^\pi \int_0^\pi \frac{\cos(mk_1)\cos(nk_2)}{t - i\varepsilon - \cos(k_1) - \cos(k_2)} \tag{7.13}$$

and for $t > 2$ can be written as the convergent Bessel integral

$$\int_0^\infty e^{-itx} J_m(x)J_n(x)dx = \frac{1}{(2t)^{m+n}t}\binom{m+n}{n} \times {}_4F_3\left[\begin{matrix} \frac{m+n+1}{2} & \frac{m+n+1}{2} & 1+\frac{m+n}{2} & 1+\frac{m+n}{2} \\ m+1 & n+1 & m+n+1 & \frac{4}{t^2}\end{matrix}\right]. \tag{7.14}$$

Here ${}_pF_q$ denotes the generalized hypergeometric function.[21] The analytic continuation to the region $0 < t < 2$ can be found[59] and yields

$$G(t;(m,n)) = \frac{(-1)^m}{2}\,{}_4F_3\left[\begin{matrix} \frac{1+m+n}{2} & \frac{1-m-n}{2} & \frac{1+m-n}{2} & \frac{1-m+n}{2} \\ 1 & \frac{1}{2} & \frac{1}{2} & \frac{t^2}{4}\end{matrix}\right] + \frac{(-1)^{m+1}(m^2-n^2)t}{4}\,{}_4F_3\left[\begin{matrix} \frac{m+n+2}{2} & \frac{m-n+2}{2} & \frac{2-m-n}{2} & \frac{2-m+n}{2} \\ 1 & \frac{3}{2} & \frac{1}{2} & \frac{t^2}{4}\end{matrix}\right] \tag{7.15}$$

if m and n have the same parity, for example. Again, the corresponding Watson integral $(t = 2, m = n = 0)$ does not exist. In three dimensions the matter is drastically more complicated, and only a few special cases have been worked out analytically. Let us look at the extended Watson integral

$$W(z) = \frac{\mathcal{P}}{\pi^3}\int_0^\pi \int_0^\pi \int_0^\pi \frac{d^3\mathbf{k}}{1 - \frac{z}{3}(\cos(k_1)+\cos(k_2)+\cos(k_3))}, \tag{7.16}$$

for which the integrand is singular for $-1 \le z \le 1$. This was evaluated by Watson[58] for $z = \pm 1$ in 1939, but in spite of numerous attempts, was not evaluated for general z until 1973 in an important paper[32] by Joyce. The following is a somewhat simplified version of his calculation.

Formally, the pole in a principal value integral can be eliminated, at the cost of an additional integration, by the identity

$$\frac{1}{x-y} = \int_0^\infty e^{-sx}e^{sy}ds\,, \tag{7.17}$$

where the convergence, if $x < y$, depends on the nature of the original integrand. By applying this to (7.13) and invoking the integral representation for the modified Bessel function, we obtain

$$W(z) = \int_0^\infty e^{-s} I_0^3(sz/3)ds. \tag{7.18}$$

Next, we use the identity[26]

$$I_0^3(x) = \sum_{k=0}^{\infty} \frac{(1/2)_k}{(2k)!k!}\, {}_3F_2[-k,-k,1/2;1,1;4]x^{2k} \tag{7.19}$$

to write $W(z) = \sum_{n=0}^{\infty} A_n z^{2n}$. The coefficients A_n, being hypergeometric, must obey a simple recursion relation,[26] which in this case is

$$\begin{aligned} 36(n+2)^3 A_{n+2} \;-\; 2(2n+3)(10n^2+30n+23)A_{n+1} \\ +\;(n+1)(4n^2+8n+3)A_n = 0. \end{aligned} \tag{7.20}$$

Identifying (7.20) as the recurrence relation arising in the series solution of a differential equation, we find that $W(z)$ must be a solution to the third-order ordinary differential equation ($x = z^2$)

$$\begin{aligned} W'''(x) + 3f(x)W''(x) + [2(f(x))^2 + f'(x) + 4g(x)]W'(x) \\ + [4f(x)g(x) + 2g'(x)]W(x) = 0, \end{aligned}$$

$$\begin{aligned} f(x) &= \frac{1}{x} + \frac{1}{2(x-1)} + \frac{1}{2(x-9)} \\ g(x) &= \frac{3(x-4)}{16x(x-1)(x-9)}. \end{aligned} \tag{7.21}$$

It is known from the theory of generalized hypergeometric equations that the solution to (7.21) regular at the origin is proportional to $[y(x)]^2$, where $y(x)$ is the regular solution to the second-order equation $y'' + f(x)y' + g(x)y = 0$. Joyce was able to identify this with Heun's equation, showing that *W(z)* is essentially the square of a Heun function. Finally, by invoking various transformation properties of Heun functions,[53] he obtained

$$\begin{aligned} W(z) &= \frac{(1-\frac{3}{4}x_1)^{1/2}}{(1-x_1)}\frac{4}{\pi^2}K(k_+)K(k_-)\,, \\ k_\pm^2 &= \frac{1}{2} \pm \frac{1}{4}x_2\sqrt{4-x_2} - \frac{1}{4}(2-x_2)\sqrt{1-x_2}\,, \end{aligned}$$

where

$$\begin{aligned} x_1 &= \frac{1}{2} + \frac{1}{6}z^2 - \frac{1}{2}\sqrt{(1-z^2)(1-\frac{1}{4}z^2)}\,, \\ x_2 &= \frac{x_1}{x_1 - 1}\,. \end{aligned} \tag{7.21}$$

Once again, one sees the striking analytic complexity unfurling from the exact resolution of a simple looking multi-dimensional PV integral.

8. Summary

In this paper, we have categorized and discussed various types of PV integrals that arise in applications. Both infinite-limit and finite-limit integrals have been examined, including comparisons for the former with complex variable theory and analyses for the latter using quadrature relations. For each of these categories we have considered the following cases:

(a) one-dimensional integrals containing a simple pole.

(b) one-dimensional integrals containing a single multiple pole.

(c) double integrals containing two simple poles.

(d) double integrals containing two multiple poles.

(e) multiple integrals containing products of simple poles.

Also, in many of these cases we have discussed or referred to various numerical methods for efficiently evaluating the integrals that occur.

In these developments we have tried to clarify certain misconceptions regarding the PV formalism. First, we have shown that the PV can be considered as the convergent part of a divergent integral. Second, we have shown how to generalize the usual definitions applicable to a single pole in a one-dimensional integral to higher order poles and multiple integrals. The role and applications of the famous PB theorem have been discussed. Third, we have shown that the value of a finite-limit PV integral can be expressed as the difference between the quadratures evaluated at the end points of the range of integration. In this regard, the PV can be viewed as the value of the integral obtained by ignoring the singularity occurring in the integrand.

Many important applications of the PV formalism have been reviewed. Various types of dispersion relations have been analyzed, including applications of the PB theorem to two- and three-particle loop integrals. The R- and T-matrix formalism in momentum space was briefly discussed. Then we have reviewed representative applications to nuclear physics, transport theory, and condensed matter physics.

Finally, various important extensions of the work should be considered in the future. One interesting idea is to attempt to evaluate the convergent part of an integral containing singularities other than poles, e.g. branch cuts. Another important application of the work might be to connect the PV formalism with the Wick rotation[31] in quantum field theory, which has been used for bound state equations in which Minkowski variables are analytically continued in order to generate a set of Euclidean coordinates.

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Appendix A. Summary of Methods for the Numerical Evaluation of PV Integrals

A number of methods have been developed for evaluating numerically a variety of PV integrals (see Refs. 10, 13, 15, 17, 29, 54, 55 and 60). Also Refs. 17, 54 and 55 contain additional references to numerical methods. In this Appendix we summarize various numerical techniques used to evaluate PV integrals.

(a) Single Integrals of the form:

$$I_1(x) = \mathcal{P} \int_0^\infty \frac{f(x')dx'}{(x'^2 - x^2)}. \tag{A.1}$$

References 10, 29 and 60 treat such integrals. In Ref. 10, a complex-plane method is used to evaluate integrals like (A.1) when $f(x)$ is a *highly oscillatory function.*

(b) Single Integrals of the form:

$$I_2(x) = \mathcal{P} \int_{-\infty}^\infty \frac{f(x')dx'}{x' - x}. \tag{A.2}$$

In Ref. 13, methods are presented for evaluating Eq. (A.2). Also, special algorithms are developed for the following cases:

(i) when $f(x)$ contains a single step function, namely

$$f(x) = \Theta(x - \mu)g(x) \tag{A.3}$$

and

(ii) when $f(x)$ contains *two symmetric* step functions:

$$f(x) = [\Theta(x - \mu) + \Theta(-x - \mu)]\, g(x). \tag{A.4}$$

Applications involving zero-temperature causal Green's functions for fermions and bosons furnish examples of Eqs. (A.3) and (A.4).[13] (See Sec. 3.1, in particular Eq. (3.3).)

(c) Single Integrals of the form:

$$I_3(x) = \mathcal{P} \int_b^c \frac{f(x')dx'}{x' - x}, \tag{A.5}$$

where b and c are finite. Algorithms for evaluating Eq. (A.5) are given in Refs. 13 and 15.

(d) Single Integrals of the form:

$$I_4(x) = \mathcal{P} \int_b^c \frac{f(x')dx'}{(x' - x)^n}, \tag{A.6}$$

where b and c are finite and $n > 1$. A method for treating this case was presented in Ref. 15. Because of the formalism developed in Sec. 2.1.3 for higher-order poles, there are boundary terms that involve derivatives of $f(x)$. Thus, in order for this numerical method to work, either these derivatives must be obtained analytically or the function $f(x)$ must be amenable to accurate numerical differentiation.

(e) Double integrals of the form:

$$I_5(u) = \int dx \frac{\mathcal{P}}{(x-u)} \int dy \frac{\mathcal{P}}{(y-x)} f(x,y), \tag{A.7}$$

where the integration limits can be either finite or infinite. The numerical evaluation of such integrals is still being perfected. Some methods for calculating integrals like Eq. (A.7) were presented in Refs. 15 and 60. Also, precision calculations of loop integrals (which involve two PV integrals, as discussed in Sec. 3.3) were discussed in Refs. 13, 14, 16 and 60.

One of the challenges of the calculation of Eq. (A.7) is to compare it with the numerical evaluation of

$$I_5'(u) = \int dy \int \frac{\mathcal{P}}{(x-u)} \frac{\mathcal{P}}{(y-x)} dx \; f(x,y) \,. \tag{A.8}$$

The difference between Eqs. (A.7) and (A.8) is the PB "interchange term" given in Eqs. (2.35) and (2.36). This interchange term vanishes if at least one of the PVs in Eqs. (A.7) or (A.8) does not occur (e.g., if the point $x = u$ is outside the range of integration). This property has been nicely demonstrated for an analytic example,[15] but it is instructive to exhibit it for cases in which the integrals must be evaluated numerically.

All numerical methods for evaluating PV integrals make use of some type of subtraction trick in order to eliminate the formal PV of the integral. In this way, we rely on the property (discussed in Sec. 2.1.4) that the PV is the convergent part of the integral. We illustrate by evaluating Eq. (A.2) or (A.5), defining[13]

$$I(a) = \mathcal{P} \int_b^c \frac{f(x)\,dx}{(x-a)}, \tag{A.9}$$

where a is real, $b < c$, and b and c are both finite or both infinite. Equation (A.7) can then be rewritten as

$$I(a) = \mathcal{P} \int_b^c \frac{[f(x) - f(a)]}{(x-a)} dx + f(a)\, \mathcal{P} \int_b^c \frac{dx}{(x-a)}. \tag{A.10}$$

Now the PV symbol can be removed in front of the first integral, so that

$$I(a) = \int_b^c \frac{[f(x) - f(a)]}{(x-a)}\, dx + f(a) \mathcal{P} \int_b^c \frac{dx}{(x-a)}. \tag{A.11}$$

If $c \to +\infty$ and $b \to -\infty$, we have from Eq. (2.62)

$$\mathcal{P} \int_{-\infty}^{\infty} \frac{dx}{x-a} = 0, \tag{A.12}$$

and if both c and b are finite

$$\mathcal{P}\int_b^c \frac{dx}{x-a} = \ln\left|\frac{c-a}{b-a}\right|, \tag{A.13}$$

a result which follows from Eq. (2.21a). Thus, the second integral in Eq. (A.9) can always be evaluated analytically.

In general, though, the first integral in Eq. (A.11) will have to be evaluated numerically. See Refs. 13 and 29 for a discussion of the types of Gaussian meshes recommended for many integrals of physical interest. (See also Eq. (B.5).) After discretizing, the first integral in Eq. (A.11) can be written as

$$\overline{I}(a) = \sum_{j=1}^{N_g} \frac{[f(x_j) - f(a)]}{(x_j - a)}\, w_j\,, \tag{A.14}$$

where N_g is the number of Gaussian points and w_j is the weight appropriate to the jth mesh point.[13,29]

However, Eq. (A.14) cannot be evaluated if a is chosen as one of the mesh points. This is a major disadvantage if we wish I and f to lie on the same mesh.[13,60] This difficulty can be overcome if $f(x)$ can be differentiated and evaluated at the mesh points (e.g. by a numerical procedure). For such cases, we find that

$$\overline{I}(x_i) = \sum_{j=1,\ j\neq i}^{N_g} \frac{[f(x_j) - f(x_i)]}{(x_j - x_i)} w_j + \left[\frac{df(x)}{dx}\right]_{x=x_i} w_i, \tag{A.15}$$

a result obtained using L'Hospital rule.[13] Unfortunately, it is not always possible to differentiate $f(x)$, particularly if $f(x)$ is a function that is not known analytically and that can only be determined by some prior numerical procedure.

Appendix B. The Haftel–Tabakin Method for Numerically Evaluating the R and T Matrices in Momentum Space

Due to Eqs. (4.5) and (4.8), we need only concern ourselves with the matrix values, $R_\ell(k, k_0)$. (That is the right-most matrix index is always k_0.) Following Haftel and Tabakin,[29] we remove the PV in the second line of Eq. (4.10) by a subtraction trick, using Eq. (2.64), obtaining

$$\begin{aligned} R_\ell(k, k_0) &= V_\ell(k, k_0) \\ &\quad - \frac{2m}{\hbar^2}\int_0^\infty \frac{dk'}{(k'^2 - k_0^2)}\left[k'^2 V_\ell(k, k')R_\ell(k', k_0) - k_0^2 V_\ell(k, k_0)R_\ell(k_0, k_0)\right]. \end{aligned} \tag{B.1}$$

The R-matrix may be evaluated by a matrix inversion[13,29,60] if Eq. (B.1) is discretized. In particular, we have

$$V_\ell(k_i, k_{N_g+1}) = \sum_{j=1}^{N_g+1} F_\ell^{(R)}(k_i, k_j)R_\ell(k_j, k_{N_g+1})\,, \tag{B.2}$$

where N_g is the order of Gaussian integration, $k_{N_g+1} \equiv k_0$, and F_ℓ is an $N_{g+1} \times N_{g+1}$ matrix defined by

$$F_\ell^{(R)}(k_i, k_j) = \delta_{ij} + \Omega_j^{(R)} V_\ell(k_i, k_j) \tag{B.3}$$

and

$$\Omega_j^{(R)} = \begin{cases} \frac{2m}{\hbar^2} w_j k_j^2/(k_j^2 - k_0^2), & \text{for } j \leq N_g. \\ -\frac{2m}{\hbar^2} k_0^2 \sum_{i=1}^{N_g} [w_i/(k_i^2 - k_0^2)] & \text{for } j = N_g + 1. \end{cases} \tag{B.4}$$

The Gaussian weight for point j is given by w_j, and the quadrature used is extracted from the transformation[13,29]

$$k_j = \tan \frac{\pi}{4}(u_j + 1), \; 1 \leq j \leq N_g, \tag{B.5}$$

where u_j is the usual Gaussian–Legendre mesh point that lies in the range $[-1, +1]$. The mesh defined by Eq. (B.5) has been widely used to evaluate many types of integrals, particularly PV integrals. Overall, it is more accurate and efficient than other quadrature schemes used for evaluating infinite-limit integrals.

By inverting Eq. (B.2), we obtain

$$R_\ell(k_i, k_{N_g+1}) = \sum_{j-1}^{N_g+1} F_\ell^{(R)-1}(k_i, k_j) \; V_\ell(k_j, k_{N_g+1}), \tag{B.6}$$

which gives the R-matrix, including the on-shell case

$$R_\ell \; (k_{N_g+1}, k_{N_g+1}) = R(k_0, k_0).$$

Clearly, in this formulation, k_0 cannot be one of the Gaussian mesh points, which may be a disadvantage in some applications. See Ref. 60 for further discussions of this problem and an alternative, approximate formulation of the method. Also, see the discussion regarding Eq. (A.14) in Appendix A.

Finally, we remark that, by comparing Eqs. (4.10) and (4.15), we can solve for the T-matrix in a similar fashion. We redefine the Ω^j in Eq. (B.4) as

$$\Omega_j^{(R)} = \begin{cases} \frac{2m}{\hbar^2} w_j k_j^2/(k_j^2 - k_0^2) & \text{for } j \leq N_g, \\ -\frac{2m}{\hbar^2} k_0^2 \sum_{i=1}^{N_g} [w_i/(k_i^2 - k_0^2)] + \frac{m\pi i}{\hbar^2} k_0^2 & \text{for } j = N_g + 1, \end{cases} \tag{B.7}$$

which gives, in Eq. (B.3), a matrix $F_\ell^{(T)}$. Then, we obtain

$$T_\ell(k_i, k_{N_g+1}) = \sum_{j=1}^{N_g+1} \left(F_\ell^{(T)}\right)^{-1} (k_i, k_j) V_\ell(k_j, k_{N_g+1}) \,. \tag{B.8}$$

Note that, if the potential V_ℓ is real, the R-matrix is also real, but the T-matrix is complex. This implies that in Sec. 4 the $\psi_\ell^{(k_0)}$ functions can be chosen real, while the $\chi_\ell^{(k_0)}$ functions are always complex. Also, the beauty of this method is that one obtains $R_\ell(k, k_0)$ and $T_\ell(k, k_0)$ for a fixed mesh of k values and, as a bonus, the "on-shell" value for $k = k_0$.

Appendix C. A Useful PV Integral Transformation

Theorem. *Let $a_j > 0$, b_j $(j = 1, \ldots, N-1)$ be any real numbers and*

$$\phi(x) = x - \sum_{j=1}^{N-1} \frac{a_j}{x - b_j}.$$

Then for any function F for which the integrals exist, and $y \neq b_j$ for any j,

$$I = \mathcal{P} \int_{-\infty}^{\infty} \frac{F[\phi(x)]}{x - y} dx = \mathcal{P} \int_{-\infty}^{\infty} \frac{F(x)}{x - \phi(y)} dx.$$

Proof. The equation $u = \phi(x)$ can be written in the form

$$G(x) / \prod_{j=1}^{N-1} (x - b_j) = 0,$$

where

$$G(x) = u \prod_{j=1}^{N-1} (x - b_j) - f(x) = \prod_{j=1}^{N} [x - x_j(u)]$$

and f is a polynomial. Here $G(x)$ has the distinct roots $x_j(u)$ which are differentiable with respect to u for $-\infty < u < \infty$. Now, for simplicity assuming that y coincides with no b_j and omitting the PV symbol on the appropriate integral,

$$I = \int_{-\infty}^{b_1^-} + \int_{b_1^+}^{b_2^-} + \cdots + \int_{b_{N-1}^+}^{\infty} \frac{F[\phi(x)]}{x - y} dx.$$

Changing the variable of integration to $x = x_j(u)$ over the range $b_{j-1} < x < b_j$, we find

$$I = \mathcal{P} \int_{-\infty}^{\infty} F(u) \sum_{j=1}^{N} \frac{x_j'(u)}{x_j - y} du.$$

But

$$\sum \frac{x_j'}{x_j - y} = \frac{d}{du} G(y) = \frac{1}{u - \phi(y)}.$$

This completes the proof.

As a simple corollary, we find that for

$$\psi(x) = \sum_{j=1}^{N-1} \frac{a_j}{x - b_j},$$

$$\mathcal{P}\int_{-\infty}^{\infty}\frac{F[\psi(x)]}{x-y}dx = \mathcal{P}\int_{-\infty}^{\infty}\frac{F(x)}{x}dx - \mathcal{P}\int_{-\infty}^{\infty}\frac{F(x)}{x-\psi(y)}dx.$$

As long as $\psi(x)$, $\phi(x)$ are convergent, N can be infinite.

As an example, take $f(x) = x(x^2+a^2)^{-1}$. Then for $\phi(x) = x - 1/x$, we find from

$$\mathcal{P}\int_{-\infty}^{\infty}\frac{x}{x^2+a^2}\frac{dx}{x-y} = \frac{\pi a}{y^2+a^2},$$

that

$$\mathcal{P}\int_{-\infty}^{\infty}\frac{x(x^2-1)}{x^4+(a^2-2)x^2+1}\frac{dx}{x-y} = \frac{\pi a^2}{y^4+(a^2-2)y^2+1}$$

which remains valid for $y=0$.

For

$$\psi(x) = x - \cot(1/x) = \frac{1}{\pi^2}\sum_{k=1}^{\infty}\frac{1}{k}\left[\frac{1}{x-(k\pi)^{-1}} + \frac{1}{x+(k\pi)^{-1}}\right],$$

we get

$$\mathcal{P}\int_{-\infty}^{\infty}\frac{x-\cot(1/x)}{[x-\cot(1/x)]^2+a^2}\frac{dx}{x-y} = \frac{\pi}{a} - \frac{\pi a}{[y-\cot(1/y)]^2+a^2}.$$

References

1. R. Balescu, **Statistical Mechanics of Changed Particles** (Interscience, 1963), p. 110.
2. R. Balescu, **Statistical Mechanics of Charged Particles** (Interscience, 1973), p. 399.
3. L. Boltzmann, *Further studies on the thermal equilibrium of gas molecules, Sitz. Wien. Akad. Wiss.* **66**, 275 (1872) (in German).
4. L. Brand, **Advanced Calculus** (John Wiley and Sons, 1955), pp. 262–264.
5. D. M. Brink and G. R. Satchler, **Angular Momentum** (Oxford Univ. Press, 1993), 3rd edition.
6. K. M. Case, *Plasma oscillations, Ann. Phys.* **9** (1960) 1–23.
7. K. M. Case, *Elementary solutions of the transport equation, Ann. Phys.* **7** (1959) 349–364.
8. K. M. Case and P. F. Zweifel, **Linear Transport Theory** (Addison-Wesley, 1967).
9. C. Cercignani, **The Boltzmann Equation and its Applications** (Springer-Verlag, 1987).
10. K. T. R. Davies, *Complex-plane methods for evaluating highly oscillatory integrals in nuclear physics:II, J. Phys.* **G14** (1988) 973–993.
11. K. T. R. Davies and R. W. Davies, *Evaluation of a class of integrals occurring in mathematical physics via a higher order generalization of the principal value, Can. J. Phys.* **67** (1989) 759–765.
12. K. T. R. Davies, R. W. Davies and G. D. White, *Dispersion relations for causal Green's functions: Derivations using the Poincaré–Bertrand theorem and its generalizations, J. Math. Phys.* **31** (1990) 1356–1373; **32** (1991) 1651(E).
13. K. T. R. Davies, G. D. White and R. W. Davies, *Evaluation of the real parts of fermion and boson propagators using dispersion relations, Nucl. Phys.* **A524** (1991) 743–767.

14. K. T. R. Davies, J. S. Wu and R. W. Davies, *Evaluation of integrals using general partial-fraction expansions*, *Can. J. Phys.* **70** (1992) 311–318.
15. K. T. R. Davies, M. L. Glasser and R. W. Davies, *Quadrature relations for finite-limit principal value integrals*, *Can. J. Phys.* **70** (1992) 656–666.
16. K. T. R. Davies, *Dyson's equations for nuclear-pion-delta interactions: Toward a self-consistent solution in nuclear matter*, *Ann. Phys.* **215** (1992) 386–456.
17. P. J. Davis and P. Rabinowitz, **Methods of Numerical Integration** (Academic Press, 1984), 2nd edition pp. 11–14 and 188–190.
18. D. F. Dubois, *Electron interactions. Part I: Field theory of a degenerate electron gas*, *Ann. Phys.* **7** (1959) 174–203.
19. J. J. Duderstadt and W. R. Martin, **Transport Theory** (J. Wiley and Sons, 1978).
20. E. Engel and S. H. Vosko, *Wave vector dependence of exchange contribution to the electron gas response functions: An analytic derivation*, *Phys. Rev.* **B42** (1990) 4949–4953.
21. A. Erdélyi, **Bateman Manuscript Project, Higher Transcendental Functions** (McGraw-Hill, 1954), Vol. I.
22. A. Erdélyi, Ed.,**Bateman Manuscript Project, Tables of Integral Transforms** (McGraw-Hill, 1954), Vol. II, pp. 243–262.
23. A. L. Fetter and J. D. Walecka, **Quantum Theory of Many Particle Systems** (McGraw-Hill, 1971), pp. 158–162, 171–197, 291–310.
24. I. M. Gel'fand and G. E. Shilov, **Generalized Functions** (Academic Press, 1964).
25. D. W. J. Geldhart and R. Taylor, *Wave-number dependence of the static screening function of an interacting electron gas. I. Lowest order Hartree-Fock correction*, *Can J. Phys.* **48** (1970) 155–165.
26. M. L. Glasser and E. Montaldi, *Staircase polygons and recurrent lattice walks*, *Phys. Rev.* **E48** (1993) R2339–R2342.
27. M. L. Glasser, *Exchange corrections to the static Lindhard screening function*, *Phys. Rev.* **B51** (1994) 7283–7286.
28. M. L. Goldberger and K. M. Watson, **Collision Theory** (John Wiley and Sons, 1964) pp. 190–192.
29. M. I. Haftel and F. Tabakin, *Nuclear saturation and the smoothness of nucleon-nucleon potentials*, *Nucl. Phys.* **A158** (1970) 1–42.
30. Eds. E. Inönü and P. F. Zweifel, **Developments in Transport Theory**, A NATO Advanced Study Institute on Transport Theory held at Ankara, Turkey (Academic Press, 1967).
31. C. Itzykson and J.-B. Zuber, **Quantum Field Theory** (McGraw-Hill, 1980), pp. 300 and 485.
32. G.S. Joyce,*On the simple cubic lattice Green function*, *Phil. Trans. Roy. Soc. (London)* **273** (1973) 583–609.
33. N. G. van Kampen, *On the theory of stationary waves in plasmas*, *Physica* **21** (1955) 949–963.
34. N. G. van Kampen, *On the problem of neutron diffusion*, *Proc. Roy. Acad. Sci. Amsterdam Ser. B* **63** (1960) 92–107.
35. M. Kirilov and M. Trott, *k-space treatment of reflection and transmission at a potential step*, *Am. J. Phys.* **62** (1994) 553–558.
36. I. Kuščer, N. J. McCormick and G. C. Summerfield, *Orthogonality of Case's eigenfunctions in one-speed transport theory*, *Ann. Phys. (N. Y.)* **30** (1964) 411–421.
37. M. J. Lighthill, **Introduction to Fourier Analysis and Generalized Functions** (Cambridge Univ. Press, 1962), pp. 34–39.

38. J. Linhard, *The properties of a gas of charged particles*, *Mat-Fys. Medd.* **28** (1954) 8–73.
39. M. H. Lee, *Solving certain principal value integrals by reduction to the dilogarithm*, to be published.
40. L. Lewin, **Dilogarithms and Associated Functions** (MacDonald & Co., 1958).
41. C. Mahaux, K. T. R. Davies and G. R. Satchler, *Retardation and dispersive effects in the nuclear mean field*, *Phys. Rep.* **224** (1993) 237–360. This review contains a number of references to applications of dispersion relations in low-energy nuclear physics.
42. A. A. Maraduddin, E. W. Montroll, G. H. Weiss and I. P. Ipatova, **Theory of Lattice Dynamics in the Harmonic Approximation** (Academic Press, 1972).
43. N. J. McCormick and I. Kuščer, *Singular eigenfunction expansions in neutron transport theory*, *Adv. Nucl. Sci. Tech.* **7** (1973) 181–282.
44. E. Merzbacher, **Quantum Mechanics** (John Wiley and Sons, 1962), pp. 501–502.
45. E. Merzbacher, **Quantum Mechanics** (John Wiley and Sons, 1962), pp. 492–494.
46. J. P. Milano and P. J. Siemens, *Model solutions of regularized relativistic transport equations*, *Phys. Rev.* **C43** (1991) 2377–2392.
47. P. M. Morse and H. Feshbach, **Methods of Theoretical Physics**, Part I (McGraw-Hill 1953), Part I, pp. 368, 370–372, 411.
48. N. I. Muskhelishvili, **Singular Integral Equations** (Noordhoff, 1953), pp. 56–61.
49. R. G. Newton and R. Shtokhamer, *Finite total three-particle scattering rates*, *Phys. Rev.* **A14** (1976) 642–657.
50. S. Paveri-Fontana and P. F. Zweifel, *The half-Hartley and the half-Hilbert transform*, *J. Math. Phys.* **35** (1994) 2648–2656.
51. S. S. Schweber, **An Introduction to Relativistic Quantum Field Theory** (Row Peterson, 1961), pp. 315-316, 328–330.
52. P. J. Siemens, M. Soyeur, G. D. White, L. J. Lantto and K. T. R. Davies, *Relativistic transport theory of fluctuating fields for hadrons*, *Phys. Rev.* **C40** (1989) 2641–2671.
53. C. Snow, **Hypergeometric and Legendre Functions** (Nat. Bureau of Standards, 1952).
54. P. S. Theocaris and N. I. Ioakimidis, *A method of numerical solution of Cauchy-type singular integral equations with generalized kernels and arbitrary complex singularities*, *J. Comput. Phys.* **30** (1979) 309–323.
55. P. S. Theocaris, N. I. Ioakimidis and J. G. Kazanzakis, *On the numerical evaluation of two-dimensional principal value integral*, *Internat. J. Numer. Methods Engrg.* **15** (1980) 629–634.
56. E. C. Titchmarsh, **Introduction to the Theory of Fourier Integrals** (Oxford Univ. Press, 1937), Theorem 95.
57. F. G. Tricomi, **Integral Equations** (Interscience, 1957), pp. 166–173.
58. G.N. Watson, *Three triple integrals*, *Quart. J. Math. Oxford* **10** (1939) 266–276.
59. G. N. Watson, **A Treatise on the Theory of Bessel Functions** (Cambridge University Press, 1966), 2nd edition.
60. G. D. White, K. T. R. Davies and P. J. Siemens, *Studies of the nuclear single-particle response function in a simple model*, *Ann. Phys.* **187** (1988) 198–246.